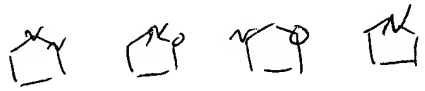
STIC Search Report
Biotech-Chem Library

STIC Database Tracking Number: 135293

TO:	From:
Rei-Tsang Shiao Location: 5a10 / 5c18 Wednesday, October 20, 2004 Art Unit: 1626 Phone: 272-0707 Serial Number: 10 / 757606	Jan Delaval Location: Biotech-Chem Library Rem 1A51 Phone: 272-2504 jan.delaval@uspto.gov

Search Notes

Robert - "Y" is unsearchable
- I had to limit "A" to:



structure is open at "A", "Y" and "AR" -

1 Hit displayed per reference
Answers saved ± 10 days if needed

FYI: pages 122 - 145 show "free" view of all hits for 10/757606

MANY excellent hits in references 1 - 41

Jan Delaval for search

Access DB# 135293

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Robert (Kent) Shiao Examiner #: 79521 Date: 10/18/04
Art Unit: 1626 Phone Number 2-0707 Serial Number: 10/757,606
Mail Box and Bldg/Room Location: 5A15/5C18 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

MEJ

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc. if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

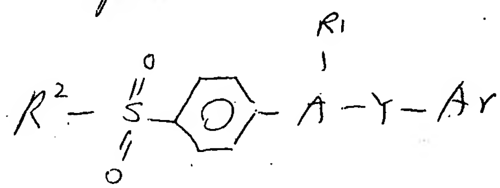
Title of invention: Substituted sulfonyl

Inventors (please provide full names): Talley et al

Earliest Priority Filing Date: __________

**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

I. search cpd I

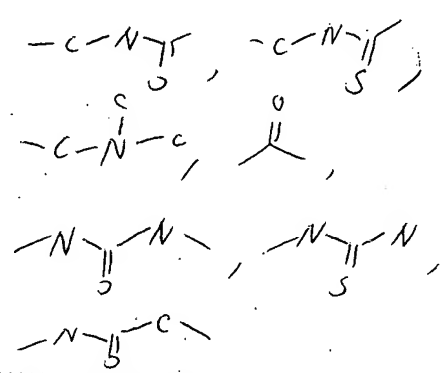


1. A is heteroaryl, or heterocycle
2. Y is a, s, N, O

3 Ar is aryl, heteroaryl,

4 R1 is sub ie, heterocycle, cycloalkyl,

5. R^2 is sub, C, N



II methods of use of cpd I.

****

STAFF USE ONLY

Searcher:	Jan	NA Sequence (#)		STN	✓
Searcher Phone #:	22504	AA Sequence (#)		Dialog	
Searcher Location:		Structure (#)	✓	Questel/Orbit	
Date Searcher Picked Up:	10/20	Bibliographic		Dr.Link	
Date Completed:	10/26	Litigation		Lexis/Nexis	
Searcher Prep & Review Time:		Fulltext		Sequence Systems	
Clerical Prep Time:	20	Patent Family		WWW/Internet	
Online Time:	±60	Other		Other (specify)	

Type of Search — Vendors and cost where applicable

PTO-1590 (8-01)

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=> fil reg
FILE 'REGISTRY' ENTERED AT 16:36:29 ON 20 OCT 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   19 OCT 2004  HIGHEST RN 765878-56-6
DICTIONARY FILE UPDATES:  19 OCT 2004  HIGHEST RN 765878-56-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> d sta que l38
L28             STR
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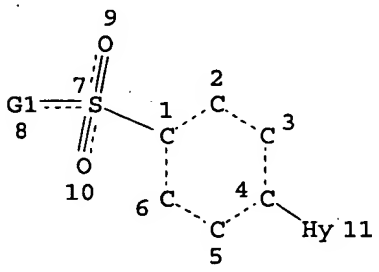


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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC   1
NUMBER OF NODES IS  11

STEREO ATTRIBUTES: NONE
L29             SCR 1840
L31      345276 SEA FILE=REGISTRY ABB=ON  PLU=ON  46.150.18/RID AND NR>=3 AND
                S/ELS AND (NC4 OR N2C3 OR NCOC2 OR NOC3)/ES
L33        6118 SEA FILE=REGISTRY SUB=L31 CSS FUL L28 AND L29
L36             STR
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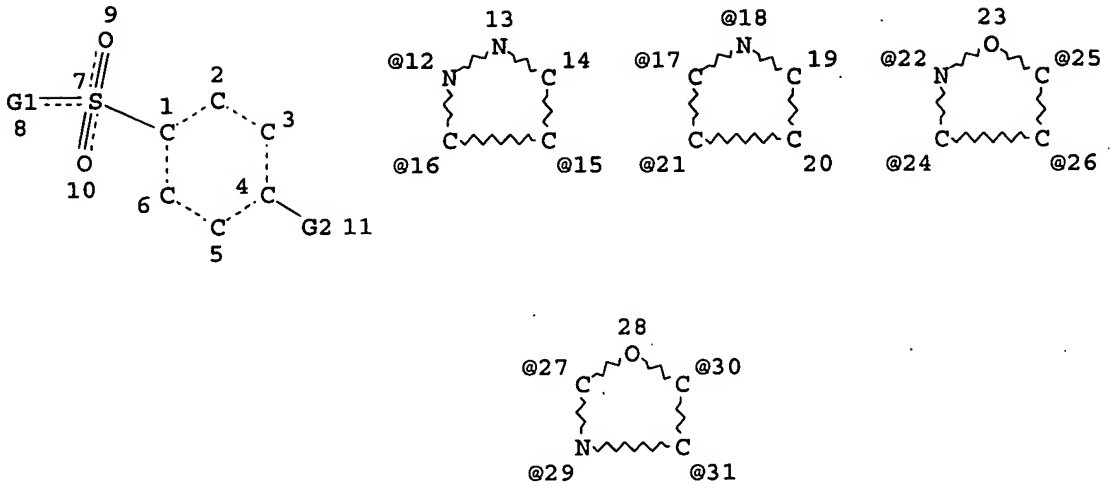

VAR G1=AK/NH2
VAR G2=12/16/15/18/17/21/22/24/26/25/29/27/31/30
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 1 12 17 22 27
NUMBER OF NODES IS 31

STEREO ATTRIBUTES: NONE
L38 5844 SEA FILE=REGISTRY SUB=L33 SSS FUL L36

100.0% PROCESSED 5996 ITERATIONS 5844 ANSWERS
SEARCH TIME: 00.00.01

=> d his

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SET COST OFF

FILE 'HCAPLUS' ENTERED AT 15:42:35 ON 20 OCT 2004
L1 1 S (US6677364 OR US2004147565)/PN OR (US2000-549830# OR US98-952
E TALLEY J/AU
L2 141 S E3,E7,E21,E24,E25
E SIKORSKI J/AU
L3 232 S E3,E4,E6-E8
E DEVADAS B/AU
L4 72 S E3-E7
E GRANETO M/AU
L5 41 S E4-E8
E CARTER J/AU
L6 114 S E3,E37
E CARTER JEF/AU
L7 44 S E4,E5,E7,E8,E9,E16
E NORMAN B/AU
L8 129 S E3
L9 56 S E35-E38
E ROGERS R/AU
L10 36 S E3,E29-E31
E ROGERS ROLAND/AU

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L11          20 S E5
                E ROGERS K/AU
L12          23 S E3,E2
L13           1 S E44
                E LU H/AU
L14         339 S E3,E8
                E LU HWANG/AU
L15          23 S E4
                E BROWN D/AU
L16         823 S E3,E39-E43
                E BROWN DAVE/AU
L17         474 S E3,E4
                E BROWN DAVID L/AU
L18         137 S E3-E10
L19        3894 S (G D SEARL?)/PA,CS
L20          21 S (GD SEARL?)/PA,CS
                E SEARLE/PA,CS
L21        4989 S E3,E4 OR SEARLE?/PA,CS
                SEL RN L1

     FILE 'REGISTRY' ENTERED AT 15:49:55 ON 20 OCT 2004
L22         112 S E1-E112
L23          56 S L22 AND 46.150.18/RID AND S/ELS AND NR>=3
L24          43 S L23 AND (NC4 OR N2C3 OR NCOC2)/ES
L25          13 S L23 NOT L24
L26           3 S L25 AND NOC3/ES
L27          46 S L24,L26
L28             STR
L29             SCR 1840
L30          16 S L28 AND L29 CSS SAM
L31      345276 S 46.150.18/RID AND NR>=3 AND S/ELS AND (NC4 OR N2C3 OR NCOC2 O
L32          50 S L28 AND L29 CSS SAM SUB=L31
L33        6118 S L28 AND L29 CSS FUL SUB=L31
                SAV TEMP L33 SHIAO757/A
L34          46 S L22 AND L33
L35          46 S L27,L34
L36             STR L28
L37          50 S L36 SAM SUB=L33
L38        5844 S L36 FUL SUB=L33
                SAV L38 TEMP SHIAO757A/A

     FILE 'HCAPLUS' ENTERED AT 16:05:05 ON 20 OCT 2004

     FILE 'REGISTRY' ENTERED AT 16:06:40 ON 20 OCT 2004
L39           1 S 80619-02-9
                E CYCLOOXYGENASE/CN
L40           3 S E3,E9,E10,E12

     FILE 'HCAPLUS' ENTERED AT 16:08:23 ON 20 OCT 2004
L41       16988 S L39 OR L40
L42        4725 S 5(1W)LIPOXYGENASE OR ARACHDION? 5 LIPOXYGENASE OR (C5 OR C 5)
L43        9691 S (CYCLOOXYGENASE OR COX)()(1 OR 2 OR 3)
L44        3312 S COX1 OR COX2 OR COX3
L45       20988 S CYCLOOXYGENASE
L46         992 S PROSTAGLANDIN H# SYNTHASE
L47         413 S CYCLO OXYGENASE()(1 OR 2 OR 3)
L48        2057 S CYCLO OXYGENASE
L49         215 S PROSTAGLANDIN G H SYNTHASE
L50          98 S PROSTAGLANDIN ENDOPEROXIDE H SYNTHASE()(1 OR 2 OR 3)
L51          71 S PROSTAGLANDIN H# SYNTHETASE
L52         182 S PROSTAGLANDIN ENDOPEROXIDE SYNTHASE()(1 OR 2 OR 3)
L53         300 S PGH SYNTHASE
                E ANTIINFLAM/CT
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                E E5+ALL
                E E2+ALL
L54         60404 S E4,E5,E3,E11-E17
                E E18+ALL
L55          9070 S E6,E5
                E E8+ALL
L56          8157 S E4
                E ANTIPYRET/CT
                E E9+ALL
L57          4667 S E3
                E E10+ALL
L58         32774 S E5
                E INFLAMMATION/CT
                E E3+ALL
L59         98093 S E2+NT
L60          6870 S E39+OLD,NT
L61         13939 S E42+OLD,NT
L62         11964 S E41+OLD,NT
                E ARTHRITIS/CT
                E E3+ALL
L63         27281 S E6+NT
L64          1823 S E23+OLD,NT
                E E5+ALL
L65          3106 S E3-E5
L66          6239 S E29+OLD,NT
                E ANALGESIA/CT
                E E3+ALL
L67          9562 S E5
                E E12+ALL
L68         17603 S E3+NT
L69          1766 S E25+OLD,NT
                E ASTHMA/CT
                E E3+ALL
L70         15672 S E9
L71           943 S E13+OLD,NT
L72         12139 S E12+OLD,NT
                E ALLERGY/CT
                E E3+ALL
L73         24276 S E3,E2+NT
L74          9185 S E15+OLD,NT
L75          1125 S E20+OLD,NT
                E PYRE/CT
                E E98+ALL
                E E2+ALL
L76          1261 S E2
L77         10401 S E5+OLD,NT
                E E5+ALL
L78          8672 S E12+OLD,NT OR E13+OLD,NT
L79           327 S L35
L80          1983 S L38
L81           298 S L79 AND L41-L78
L82          1305 S L80 AND L41-L78
L83            77 S L81,L82 AND L1-L21
L84            35 S L83 AND (PD<=19960531 OR PRD<=19960531 OR AD<=19960531)
L85            35 S L1,L84
L86          1228 S L81,L82 NOT L83
L87            48 S L86 AND (PD<=19960531 OR PRD<=19960531 OR AD<=19960531)
L88           299 S L35 (L) (THU OR DMA OR PAC OR PKT OR BAC)/RL
L89          1361 S L38 (L) (THU OR DMA OR PAC OR PKT OR BAC)/RL
L90            18 S L85 AND L88
L91            28 S L87 AND L89
L92            46 S L90,L91
L93            17 S L85 NOT L92
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L94          20 S L87 NOT L92
                SEL DN AN L93 1 2 3 5 7 10 11 12 17
L95           8 S L93 NOT E1-E27
                SEL DN AN L90 10 11 12
L96          15 S L90 NOT E28-E36
L97          23 S L95,L96
                SEL DN AN L91 6-10  18 19 20 21 22 23 24 25 27
L98          14 S L91 AND E37-E78
L99          37 S L97,L98
L100         46 S L92-L98 NOT L99
                SEL DN AN 19 21 25 39
L101          4 S L100 AND E79-E90
L102         41 S L99,L101 AND L1-L21,L41-L101

     FILE 'REGISTRY' ENTERED AT 16:36:29 ON 20 OCT 2004

=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 16:36:51 ON 20 OCT 2004
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FILE COVERS 1907 - 20 Oct 2004  VOL 141 ISS 17
FILE LAST UPDATED: 19 Oct 2004  (20041019/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=> d l102 all fhitstr tot

L102 ANSWER 1 OF 41  HCAPLUS  COPYRIGHT 2004 ACS on STN
AN   2002:942791  HCAPLUS
DN   138:14058
ED   Entered STN:  12 Dec 2002
TI   Preparation of pyrazolylbenzenesulfonamides as cyclooxygenase
     inhibitors for treatment of inflammation.
IN   Talley, John J.; Penning, Thomas D.; Collins, Paul W.; Rogier,
     Donald J., Jr.; Malecha, James W.; Miyashiro, Julie M.; Bertenshaw,
     Stephen R.; Khanna, Ish K.; Graneto, Matthew J.; Rogers,
     Roland S.; Carter, Jeffery S.; Docter, Stephen H.; Yu,
     Stella S.
PA   G.D. Searle and Co., USA
SO   U.S., 55 pp., Cont.-in-part of U.S. 6,413,960.
     CODEN: USXXAM
DT   Patent
LA   English
IC   ICM  A61P029-00
NCL  514406000; 514236500
CC   28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
     Section cross-reference(s): 1
FAN.CNT 4
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	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	US 6492411	B1	20021210	US 2002-125325	20020417	<--
	US 5466823	A	19951114	US 1993-160594	19931130	<--
	US 5521207	A	19960528	US 1994-223629	19940406	<--
	WO 9515316	A1	19950608	WO 1994-US12720	19941114	<--
	W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, US					
	RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
	US 5760068	A	19980602	US 1996-648113	19960906	<--
	US 6156781	A	20001205	US 1999-449076	19991124	<--
	US 6413960	B1	20020702	US 2000-609011	20000530	<--
	US 6586603	B1	20030701	US 2002-274679	20021021	<--
	US 6716991	B1	20040406	US 2003-378781	20030304	<--
	US 2004192930	A1	20040930	US 2003-700019	20031103	<--
PRAI	US 1993-160594	A2	19931130	<--		
	US 1994-223629	A1	19940406	<--		
	WO 1994-US12720	A1	19941114	<--		
	US 1996-648113	A1	19960906			
	US 1997-957345	B1	19971024			
	US 1999-449076	A1	19991124			
	US 2000-609011	A2	20000530			
	US 2002-125325	A1	20020417			
	US 2002-274679	A1	20021021			
	US 2003-378781	A1	20030304			

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES	
US 6492411	ICM	A61P029-00	
	NCL	514406000; 514236500	
US 6492411	ECLA	C07D231/12B3; C07D231/12B5; C07D231/14; C07D231/16; C07D231/54; C07D401/04; C07D403/0; C07D405/04; C07D405/04; C07D405/04; C07D409/04; C07D495/04	<--
US 5466823	ECLA	C07D231/12B3; C07D231/12B5; C07D231/14; C07D231/16; C07D231/54; C07D401/04; C07D405/0; C07D405/04; C07D405/04; C07D409/04; C07D409/04;	<--
US 5521207	ECLA	C07D231/12B3; C07D231/12B5; C07D231/14; C07D231/16; C07D231/54; C07D401/04; C07D405/0; C07D405/04; C07D405/04; C07D409/04; C07D409/04;	<--
US 6413960	ECLA	C07D231/12B3; C07D231/12B5; C07D231/14; C07D231/16; C07D231/54; C07D401/04; C07D403/0; C07D405/04; C07D405/04; C07D405/04; C07D409/04; C07D495/04	<--
US 6586603	ECLA	C07D231/12B3; C07D231/16; C07D231/54; C07D401/04; C07D403/04; C07D405/04; C07D405/04; C07D405/04; C07D409/04; C07D409/04; C07D495/0; C07D231/12B5; C07D231/14	<--
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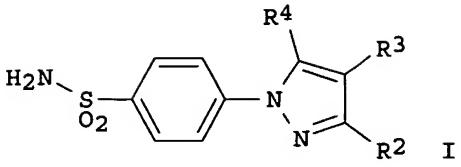
OS MARPAT 138:14058

GI



I

AB A method for the treatment of headache comprises administration of an asthma treating-effective amount of title compds. [I; R2 = H, alkyl, haloalkyl, alkoxycarbonyl, cyano, cyanoalkyl, CO2H, aminocarbonyl, alkylaminocarbonyl, cycloalkylaminocarbonyl, arylaminocarbonyl, carboxyalkylaminocarbonyl, carboxyalkyl, aralkoxycarbonylalkylaminocarbonyl, aminocarbonylalkyl, alkoxycarbonylcyanoalkenyl hydroxyalkyl; R3 = H, alkyl, cyano, hydroxyalkyl, cycloalkyl, alkylsulfonyl, halo; R4 = aralkenyl, aryl, cycloalkyl, cycloalkenyl heterocyclic; R4 is optionally substituted with ≥1 of alkylthio, alkylsulfonyl, cyano, nitro, haloalkyl, alkyl, OH, alkenyl, hydroxyalkyl, CO2H, cycloalkyl, alkylamino, dialkylamino, alkoxycarbonyl, aminocarbonyl, alkoxy, haloalkoxy, sulfamyl, heterocyclyl, amino; provided R2 and R3 are not both H; further provided that R2 ≠ CO2H or Me when R3 = H and when R4 = Ph; further provided that R4 ≠ triazolyl when R2 = Me; further provided that R4 ≠ aralkenyl when R2 = carboxyl, aminocarbonyl, ethoxycarbonyl; further provided that R4 ≠ Ph when R2 = Me and R3 = CO2H; and further provided that R4 ≠ unsubstituted thienyl when R2 = CF3], is claimed. Thus, 4,4,4-trifluoro-1-[4-(chloro)phenyl]butane-1,3-dione (preparation given) 4-sulfonamidophenylhydrazine hydrochloride were refluxed 20 h in EtOH to give 4-[5-(4-chlorophenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide. The latter at 10 mg/kg gave 44% inhibition in the rat paw edema test.

ST pyrazolylbenzenesulfonamide prepn **cyclooxygenase** inhibitor antiinflammatory; headache treatment pyrazolylbenzenesulfonamide

IT **Analgesics**
Anti-inflammatory agents
Antiasthmatics
Human
(preparation of pyrazolylbenzenesulfonamides as **cyclooxygenase** inhibitors for treatment of inflammation)

IT **Asthma**
Headache
(treatment; preparation of pyrazolylbenzenesulfonamides as **cyclooxygenase** inhibitors for treatment of inflammation)

IT **329900-75-6, Cyclooxygenase-2**
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(inhibitors; preparation of pyrazolylbenzenesulfonamides as **cyclooxygenase** inhibitors for treatment of inflammation)

IT **170570-80-6P 170570-84-0P**
RL: **PAC (Pharmacological activity)**; RCT (Reactant); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of pyrazolylbenzenesulfonamides as **cyclooxygenase** inhibitors for treatment of inflammation)

IT **970-12-7P 169590-41-4P 169590-42-5P,**
4-[5-(4-Methylphenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide **170569-22-9P 170569-23-0P**
170569-25-2P 170569-26-3P 170569-27-4P
170569-28-5P 170569-29-6P 170569-30-9P
170569-31-0P 170569-32-1P 170569-33-2P
170569-34-3P 170569-35-4P 170569-36-5P
170569-37-6P 170569-38-7P 170569-39-8P
170569-40-1P 170569-41-2P 170569-42-3P

170569-43-4P 170569-44-5P 170569-45-6P
170569-46-7P 170569-47-8P 170569-48-9P
170569-49-0P 170569-50-3P 170569-51-4P
170569-52-5P 170569-53-6P 170569-54-7P
170569-55-8P 170569-56-9P 170569-57-0P
170569-58-1P 170569-60-5P 170569-61-6P
170569-62-7P 170569-63-8P 170569-64-9P
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170569-68-3P 170569-69-4P 170569-70-7P
170569-71-8P 170569-72-9P 170569-73-0P
170569-74-1P 170569-75-2P 170569-76-3P
170569-77-4P 170569-78-5P 170569-79-6P
170569-80-9P 170569-81-0P 170569-83-2P
170569-84-3P 170569-85-4P 170569-86-5P,
4-[5-(4-Chlorophenyl)-3-(trifluoromethyl)-1H-pyrazol-1-
yl]benzenesulfonamide 170569-87-6P 170569-88-7P
170569-89-8P 170569-90-1P 170569-91-2P
170569-92-3P 170569-93-4P 170569-94-5P
170569-95-6P 170569-96-7P 170569-97-8P
170569-98-9P 170569-99-0P 170570-00-0P
170570-01-1P 170570-02-2P 170570-03-3P
170570-04-4P 170570-05-5P 170570-06-6P
170570-07-7P 170570-08-8P 170570-09-9P
170570-10-2P 170570-11-3P 170570-12-4P
170570-13-5P 170570-14-6P 170570-15-7P
170570-16-8P 170570-17-9P, 4-[5-(3-Ethyl-4-
methoxyphenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide
170570-18-0P 170570-19-1P, 4-[5-[3-(2-Propen-1-yl)-4-
methoxyphenyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide
170570-20-4P, 4-[5-(3,5-Dichloro-4-methoxyphenyl)-3-
(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide 170570-21-5P
170570-22-6P 170570-23-7P, 4-[5-(3-Methyl-4-
methylthiophenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide
170570-24-8P 170570-25-9P 170570-26-0P,
4-[5-(4-Methyl-3-nitrophenyl)-3-(trifluoromethyl)-1H-pyrazol-1-
yl]benzenesulfonamide 170570-27-1P 170570-28-2P,
4-[5-(3-Amino-4-methylphenyl)-3-(trifluoromethyl)-1H-pyrazol-1-
yl]benzenesulfonamide 170570-29-3P 170570-30-6P
170570-31-7P 170570-32-8P 170570-33-9P
170570-34-0P 170570-35-1P 170570-36-2P
170570-37-3P 170570-38-4P 170570-39-5P
170570-40-8P 170570-41-9P 170570-42-0P
170570-43-1P 170570-44-2P 170570-45-3P
170570-46-4P 170570-47-5P 170570-49-7P
170570-50-0P 170570-51-1P 170570-52-2P
170570-53-3P 170570-54-4P 170570-55-5P
170570-56-6P 170570-57-7P 170570-58-8P
170570-59-9P 170570-60-2P 170570-61-3P
170570-62-4P 170570-63-5P 170570-64-6P
170570-65-7P 170570-66-8P 170570-68-0P
170570-72-6P 170570-73-7P 170570-97-5P,
4-[5-(3-Propyl-4-methoxyphenyl)-3-(trifluoromethyl)-1H-pyrazol-1-
yl]benzenesulfonamide 170570-98-6P, 4-[5-(3-Cyclopropylmethyl-4-
methoxyphenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide
170571-00-3P, 4-[5-(4-Hydroxymethylphenyl)-3-(trifluoromethyl)-1H-
pyrazol-1-yl]benzenesulfonamide 170571-01-4P,
4-[1-[4-(Aminosulfonyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]benzoic
Acid 170571-02-5P 170571-04-7P 170571-05-8P
170571-06-9P 170571-07-0P 170571-08-1P
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170571-85-4P 170571-86-5P 170571-87-6P 170571-88-7P 170571-89-8P
170571-90-1P 170571-91-2P **170571-92-3P**
RL: **PAC (Pharmacological activity)**; SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolylbenzenesulfonamides as **cyclooxygenase** inhibitors for treatment of inflammation)

IT **170571-93-4P 170571-94-5P 170571-95-6P**
170571-96-7P 170571-97-8P 170571-98-9P
170571-99-0P 170572-00-6P 170572-01-7P
170572-02-8P 170572-03-9P 170572-04-0P
170572-05-1P 170572-06-2P 170572-07-3P
170572-08-4P 170572-09-5P **170572-10-8P** 170572-11-9P
170572-13-1P 170572-15-3P 188816-93-5P
189346-78-9P 189346-80-3P
RL: **PAC (Pharmacological activity)**; SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolylbenzenesulfonamides as **cyclooxygenase** inhibitors for treatment of inflammation)

IT **188816-86-6 374591-29-4 377091-43-5**
477801-62-0 477801-63-1 477801-64-2
477801-65-3 477801-66-4 477801-67-5
477801-68-6 477801-69-7 477801-70-0
477801-71-1 477801-72-2 477801-73-3
477801-74-4 477801-75-5 477801-76-6
477801-77-7 477801-78-8 477801-79-9
477801-80-2 477801-81-3 477801-82-4
477801-83-5 477801-84-6 477801-85-7
RL: **PAC (Pharmacological activity)**; **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(preparation of pyrazolylbenzenesulfonamides as **cyclooxygenase** inhibitors for treatment of inflammation)

IT 75-36-5, Acetyl chloride 93-55-0, Propiophenone 96-48-0, γ-Butyrolactone 98-86-2, Acetophenone, reactions 99-91-2, 4'-Chloroacetophenone 100-06-1 106-31-0, Butyric anhydride 108-42-9, 3-Chloroaniline 109-94-4, Ethyl formate 118-93-4 122-00-9, 4'-Methylacetophenone 137-06-4, o-Thiocresol 321-28-8, 2-Fluoroanisole 356-27-4, Ethyl heptafluorobutyrate 383-63-1, Ethyl trifluoroacetate 403-42-9, 4'-Fluoroacetophenone 437-82-1, 2,6-Difluoroanisole 454-31-9, Ethyl difluoroacetate 488-17-5, 3-Methylcatechol 529-34-0, 1-Tetralone 553-90-2, Dimethyl oxalate 578-58-5, 2-Methylanisole 1132-05-4, 3-Allyl-4-hydroxyacetophenone 1514-87-0, Methyl 2-chloro-2,2-difluoroacetate 1565-17-9, 4-Aminosulfonylacetophenone

1984-65-2, 2,6-Dichloroanisole 2746-25-0, 4-Methoxybenzyl bromide 2892-18-4, 5-Methyl-1-phenyl-1-hexen-3-one 3162-29-6 4653-11-6, 4-(2-Thienyl)butyric acid 7051-34-5, Bromomethylcyclopropane 14804-32-1, 2-Ethylanisole 22047-25-2, Acetylpyrazine 27918-19-0, 4-Sulfonamidophenylhydrazine hydrochloride 51015-29-3, 6-Methyltetral-1-one 170570-78-2, 1-(1,3-Benzodioxol-5-yl)-4,4-difluorobutane-1,3-dione 170570-82-8, 4,4-Dichloro-1-(3-fluoro-4-methoxyphenyl)butane-1,3-dione **170570-83-9 170570-88-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrazolylbenzenesulfonamides as **cyclooxygenase** inhibitors for treatment of inflammation)

IT 318-46-7P, 2-Trifluoroacetyl-1-tetralone 322-06-5P, 2-Methyl-1-phenyl-4,4,4-trifluorobutane-1,3-dione 326-06-7P, 4,4,4-Trifluoro-1-phenylbutane-1,3-dione 450-95-3P, 2-Fluoroacetophenone 455-91-4P, 3'-Fluoro-4'-methoxyacetophenone 720-94-5P, 1-(4-Methylphenyl)-4,4,4-trifluorobutane-1,3-dione 2388-73-0P, 2-Methylthioanisole 6739-22-6P 13414-95-4P, 4-keto-4,5,6,7-Tetrahydrothianaphthene 15191-68-1P, 4,4,4-Trifluoro-1-(4-methoxyphenyl)butane-1,3-dione 18931-60-7P, 4,4,4-Trifluoro-1-[4-(chloro)phenyl]butane-1,3-dione 20487-10-9P, 4-Methyl-1,3-benzodioxole 20577-73-5P, Methyl 4-phenyl-2,4-dioxobutanoate 29643-34-3P 29665-52-9P 39757-34-1P, Methyl 4-[4-fluorophenyl]-2,4-dioxobutanoate 39757-35-2P, Methyl 4-[4-(chloro)phenyl]-2,4-dioxobutanoate 56856-73-6P, 3-[4-(Chloro)phenyl]-propane-1,3-dione 63301-25-7P 74457-86-6P, 2'-Fluoro-4'-methoxyacetophenone 100256-35-7P, 3-Propyl-4-methoxyacetophenone 106876-38-4P, 4,4,5,5,6,6,6-Heptafluoro-1-[4-(chloro)phenyl]hexane-1,3-dione 142499-46-5P, 3-Allyl-4-methoxyacetophenone 164342-68-1P, 4-Chloro-4,4-difluoro-1-[4-(chloro)phenyl]-butane-1,3-dione 170570-76-0P, 4,4-Difluoro-[4-(chloro)phenyl]-butane-1,3-dione 170570-77-1P, 4,4-Difluoro-1-(3-fluoro-4-methoxyphenyl)-butane-1,3-dione 170570-79-3P, 3,5-Difluoro-4-methoxyacetophenone **170570-81-7P** 170570-85-1P, 4,4-Difluoro-1-(2-pyrazinyl)-butane-1,3-dione 170570-86-2P, 5-Acetyl-4-methyl-1,3-benzodioxole 170570-89-5P 170570-90-8P **170570-91-9P**, 4-[5-(4-Chlorophenyl)-1H-pyrazol-1-yl]benzenesulfonamide **170570-94-2P** 170570-95-3P, N,N-Bis(4-methoxybenzyl)-4-(aminosulfonyl)acetophenone 170570-96-4P 189347-36-2P, 3-Cyclopropylmethyl-4-methoxyacetophenone **189347-54-4P** 477801-61-9P, 3,5-Difluoro-4-acetoxyacetophenone
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrazolylbenzenesulfonamides as **cyclooxygenase** inhibitors for treatment of inflammation)

RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD

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IT **329900-75-6, Cyclooxygenase-2**
RL: **PAC (Pharmacological activity); THU (Therapeutic use); THU (Therapeutic use); THU (Therapeutic use)**
(inhibitors; preparation of pyrazolylbenzenesulfonamides as **cyclooxygenase** inhibitors for treatment of inflammation)
RN 329900-75-6 HCAPLUS
CN Synthetase, prostaglandin endoperoxide, 2 (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L102 ANSWER 2 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN **2002:172487** HCAPLUS
DN **136:221745**
ED Entered STN: 08 Mar 2002
TI Irrigation solution and method for inhibition of pain and inflammation
IN Demopulos, Gregory A.; Pierce-Palmer, Pamela; Herz, Jeffrey M.
PA Omeros Medical Systems, USA
SO U.S. Pat. Appl. Publ., 58 pp., Cont.-in-part of Appl. No. PCT/US99/24625.
CODEN: USXXCO
DT Patent
LA English
IC ICM A61K031-4427
ICS A61K031-4439; A61K031-55
NCL 514210200
CC 63-6 (Pharmaceuticals)
Section cross-reference(s): 1
FAN.CNT 14

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2002028798	A1	20020307	US 2001-839633	20010420 <--
	WO 9619233	A2	19960627	WO 1995-US16028	19951212 <--
	WO 9619233	A3	19960919		
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	WO 2000023061	A2	20000427	WO 1999-US24557	19991020
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	WO 2000023062	A2	20000427	WO 1999-US24558	19991020
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    AU 2000011277        A5    20000508    AU 2000-11277          19991020
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CLASS
 PATENT NO.       CLASS  PATENT FAMILY CLASSIFICATION CODES
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 US 2002028798    ICM    A61K031-4427
                  ICS    A61K031-4439; A61K031-55
                  NCL    514210200
 WO 9619233       ECLA   A61K038/57; A61K038/58; A61K045/06; A61K045/06;
                         A61K031/00; A61K031/4045; A61K031/48; A61K038/04;
                         A61K038/04T; A61K038/06; A61K038/08; A61K038/12;
                         A61K038/17A2; A61K038/22; A61K038/22G; A61K038/22G  <--
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US 5820583 ECLA A61K031/00; A61K031/4045; A61K031/48; A61K038/04; A61K038/04T; A61K038/06; A61K038/08; A61K038/17A2; A61K038/22; A61K038/22G; A61K038/22G; A61K038/57; A61K038/58; A61K045/06 <--
US 2003087962 ECLA A61K031/00; A61K031/18; A61K031/352; A61K031/4164; A61K031/4168; A61K031/4174; A61K031/439; A61K003/4406; A61K031/4427; A61K031/4439; A61K031/444; A61K031/498; A61K031/538; A61K031/55; A61K045/06
US 2003096807 ECLA A61K031/00; A61K031/18; A61K031/352; A61K031/4164; A61K031/4168; A61K031/4174; A61K031/439; A61K003/4406; A61K031/4427; A61K031/4439; A61K031/444; A61K031/498; A61K031/538; A61K031/55; A61K045/06

AB A method and solution for perioperatively inhibiting a variety of pain and inflammation processes at wounds from general surgical procedures including oral/dental procedures. The solution preferably includes at least one pharmacol. agent selected from the group consisting of a mitogen-activated protein kinase (MAPK) inhibitor, an α2-receptor agonist, a neuronal nicotinic acetylcholine receptor agonist, a **cyclooxygenase-2** (**COX-2**) inhibitor, a soluble receptor and mixts. thereof, and optionally addnl. multiple pain and inflammation inhibitory agents at dilute concentration in a physiol. carrier, such as saline or lactated Ringer's solution The solution is applied by continuous irrigation of a wound during a surgical procedure for preemptive inhibition of pain and while avoiding undesirable side effects associated with oral, i.m., s.c. or i.v. application of larger doses of the agents.

ST irrigation soln analgesic antiinflammatory

IT Tachykinin receptors
(NK1 antagonists; irrigation solution for inhibition of pain and inflammation at wounds during surgical procedures)

IT Tachykinin receptors
(NK2 antagonists; irrigation solution for inhibition of pain and inflammation at wounds during surgical procedures)

IT Purinoceptor antagonists
(P2X; irrigation solution for inhibition of pain and inflammation at wounds during surgical procedures)

IT Bradykinin receptors
Calcitonin gene-related peptide receptors
Interleukin receptors
Prostanoid receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(antagonists; irrigation solution for inhibition of pain and inflammation at wounds during surgical procedures)

IT Ion channel blockers
(calcium; irrigation solution for inhibition of pain and inflammation at wounds during surgical procedures)

IT Cytokine receptors
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(class I; irrigation solution for inhibition of pain and inflammation at wounds during surgical procedures)

IT 5-HT agonists
5-HT antagonists
Analgesics
Anti-inflammatory agents
Antihistamines
Leukotriene antagonists
Nicotinic agonists
Purinoceptor agonists
Purinoceptor antagonists
Surgery
Wound

(irrigation solution for inhibition of pain and inflammation at wounds during surgical procedures)

IT Interleukin 1 receptors
Opioids
Tumor necrosis factor receptors
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(irrigation solution for inhibition of pain and inflammation at wounds during surgical procedures)

IT Leukotriene receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(leukotriene B4, antagonists; irrigation solution for inhibition of pain and inflammation at wounds during surgical procedures)

IT Leukotriene receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(leukotriene D4, antagonists; irrigation solution for inhibition of pain and inflammation at wounds during surgical procedures)

IT Ion channel openers
(potassium, ATP-sensitive; irrigation solution for inhibition of pain and inflammation at wounds during surgical procedures)

IT **Receptors**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(soluble; irrigation solution for inhibition of **pain** and inflammation at wounds during surgical procedures)

IT Drug delivery systems
(solns.; irrigation solution for inhibition of pain and inflammation at wounds during surgical procedures)

IT Blood vessel, disease
(spasm, inhibition of; irrigation solution for inhibition of pain and inflammation at wounds during surgical procedures)

IT Prostanoid receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(type EP1, antagonists; irrigation solution for inhibition of pain and inflammation at wounds during surgical procedures)

IT Prostanoid receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(type EP4, antagonists; irrigation solution for inhibition of pain and inflammation at wounds during surgical procedures)

IT Cytotoxic agents
(tyrphostins; irrigation solution for inhibition of pain and inflammation at wounds during surgical procedures)

IT Opioids
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(κ-; irrigation solution for inhibition of pain and inflammation at wounds during surgical procedures)

IT Adrenoceptor agonists
(α2-; irrigation solution for inhibition of pain and inflammation at wounds during surgical procedures)

IT Opioids
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(δ-; irrigation solution for inhibition of pain and inflammation at wounds during surgical procedures)

IT Opioids
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(μ-; irrigation solution for inhibition of pain and inflammation at wounds during surgical procedures)

IT 9029-60-1, Lipoxygenase 9043-29-2, Phospholipase A1 **39391-18-9**, **Cyclooxygenase** 142243-02-5, Mitogen-activated protein kinase **329900-75-6**, **Cyclooxygenase 2**

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(inhibitors; irrigation solution for inhibition of pain and inflammation at wounds during surgical procedures)

IT 9001-01-8, Kallikrein
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(inhibitors; irrigation solution for inhibition of pain and inflammation at wounds during surgical procedures)

IT 50-48-6, Amitriptyline 91-84-9, Mepyramine 146-48-5, Yohimbine 342-10-9, Kallidin 364-62-5, Metoclopramide 437-38-7, Fentanyl 1491-59-4, Oxymetazoline 4205-90-7, Clonidine 9087-70-1, Aprotinin 15307-86-5, Diclofenac 15585-43-0, RJR 2403 19794-93-5, Trazodone 21829-25-4, Nifedipine 33876-97-0, SIN-1 36067-72-8, BHT933 36085-73-1, BHT920 50679-08-8, Terfenadine 51803-78-2, Nimesulide 59803-98-4, UK14304 60634-51-7, LY 53857 63675-72-9, Nisoldipine 64285-06-9, (+)-Anatoxin-A 71125-38-7, Meloxicam 74103-06-3, Ketorolac 80937-31-1, Flosulide 88149-94-4, DuP 697 91147-45-4, AGN-191103 92142-32-0 100449-06-7, A-54741 103628-46-2, Sumatriptan 113563-71-6, (R)-Pinacidil 113775-47-6, Dexmedetomidine 123653-11-2, N-[2-(Cyclohexyloxy)-4-nitrophenyl]methanesulfonamide 128270-60-0, Hirulog 129623-01-4, GR82334 133052-90-1, GF 109203X 136553-81-6, BQ 123 137431-04-0, NS-49 138472-01-2, NOR-3 138614-30-9, Hoe 140 142001-63-6, SR 48968 146535-11-7, AG1296 149017-66-3, PPADS 152121-30-7 152121-47-6 152121-53-4 155262-40-1, AGN 192172 156223-05-1, GTS-21 158205-05-1, L-745337 158959-32-1, SC-57666 161416-43-9, A 84543 161416-98-4, A-85380 161417-03-4, ABT-089 **162054-19-5** 162626-99-5, FR 144420 167869-21-8 168433-84-9, SC-58451 **169590-42-5**, Celecoxib 179382-91-3, RS-57067 188627-80-7, Integrelin 189319-35-5 198283-73-7, ABT-594 203564-57-2 340830-03-7, Receptor tyrosine kinase 402850-66-2, SBI 1765F
RL: **PAC (Pharmacological activity)**; **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(irrigation solution for inhibition of pain and inflammation at wounds during surgical procedures)

IT 168570-37-4, AGN 193080
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(irrigation solution for inhibition of pain and inflammation at wounds during surgical procedures)

IT 63551-76-8
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(γ, inhibitors; irrigation solution for inhibition of pain and inflammation at wounds during surgical procedures)

IT **39391-18-9**, **Cyclooxygenase**
RL: **PAC (Pharmacological activity)**; **THU (Therapeutic use)**
(inhibitors; irrigation solution for inhibition of pain and inflammation at wounds during surgical procedures)

RN 39391-18-9 HCAPLUS
CN Synthetase, prostaglandin endoperoxide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L102 ANSWER 3 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:84600 HCAPLUS
DN 136:151161
ED Entered STN: 31 Jan 2002
TI Preparation of 4-(heterocyclyl)benzenesulfonamides as components of a combination of a **cyclooxygenase-2** inhibitors and a leukotriene B4 receptor antagonist
IN Isakson, Peter C.; Anderson, Gary D.; Gregory, Susan A.
PA **G.D. Searle** and Co., USA
SO U.S., 19 pp., Cont.-in-part of U.S. Ser. No. 489,415, abandoned.
CODEN: USXXAM

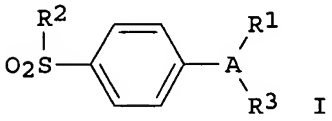
DT Patent
LA English
IC ICM A61K031-415
ICS C07D231-02; C07D231-12
NCL 514326000
CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	US 6342510	B1	20020129	US 1996-661641	19960611	<--
	CA 2224563	AA	19961227	CA 1996-2224563	19960611	<--
	US 2002107276	A1	20020808	US 2002-38080	20020103	<--
PRAI	US 1995-489415	B2	19950612	<--		
	US 1996-661641	A1	19960611			

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 6342510	ICM	A61K031-415
	ICS	C07D231-02; C07D231-12
	NCL	514326000
US 2002107276	ECLA	A61K045/06 <--

OS MARPAT 136:151161
GI



I

AB The title compds. [I; A = (partially) unsatd. heterocyclyl or carbocyclyl; R1 = (un)substituted heterocyclyl, cycloalkyl, cycloalkenyl, aryl; R2 = Me, NH2; R3 = H, halo, alkyl, etc.] which are **cyclooxygenase-2** inhibitors used in combination with a leukotriene B4 receptor antagonists for treatment of inflammation and inflammation-related disorders, were prepared and formulated. Thus, treating Et trifluoroacetate with NaOMe in Me tert-Bu ether followed by addition of 4'-chloroacetophenone (85%), and reacting the resulting 4,4,4-trifluoro-1-(4-chlorophenyl)butane-1,3-dione with 4-sulfonamidophenylhydrazine hydrochloride in EtOH afforded 4-[5-(4-chlorophenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide (80%).

ST heterocyclylbenzenesulfonamide prepn **cyclooxygenase COX2** inhibitor combination leukotriene B4; antiarthritic heterocyclylbenzenesulfonamide prepn; antiinflammatory heterocyclylbenzenesulfonamide prepn

IT Leukotriene receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(leukotriene B4; preparation of 4-(1H-pyrazol-1-yl)benzenesulfonamides as antiinflammatories)

IT **Anti-inflammatory agents**
Antiarthritics
(preparation of 4-(1H-pyrazol-1-yl)benzenesulfonamides as antiinflammatories)

IT **329900-75-6, Cyclooxygenase-2**
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of 4-(1H-pyrazol-1-yl)benzenesulfonamides as antiinflammatories)

IT **93014-16-5P**, 4-[2-Methyl-4-phenyl-5-oxazolyl]benzenesulfonamide **169590-41-4P**, 4-[5-(3-Fluoro-4-methoxyphenyl)-3-(difluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide **169590-42-5P**,

4-[5-(4-Methylphenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide **170569-86-5P**, 4-[5-(4-Chlorophenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide 177660-80-9P, 2-Methyl-5-[1-[4-(methylsulfonyl)phenyl]-4-trifluoromethyl-1H-imidazol-2-yl]pyridine 177660-92-3P, 4-[2-(5-Methylpyridin-3-yl)-4-(trifluoromethyl)-1H-imidazol-1-yl]benzenesulfonamide **181695-72-7P**, 4-[5-Methyl-3-phenylisoxazol-4-yl]benzenesulfonamide **185344-51-8P**, 4-[2-Trifluoromethyl-5-(3,4-difluorophenyl)-4-oxazolyl]benzenesulfonamide **185344-55-2P**, 4-[2-Trifluoromethyl-5-(3-fluoro-4-methoxyphenyl)-4-oxazolyl]benzenesulfonamide **195061-34-8P**
RL: **PAC (Pharmacological activity)**; SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 4-(1H-pyrazol-1-yl)benzenesulfonamides as antiinflammatories)

IT 99-91-2, 4'-Chloroacetophenone 321-28-8, 2-Fluoroanisole 383-63-1, Ethyl trifluoroacetate 454-31-9, Ethyl difluoroacetate 27918-19-0, 4-Sulfonamidophenylhydrazine hydrochloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 4-(1H-pyrazol-1-yl)benzenesulfonamides as antiinflammatories)

IT 455-91-4P, 3'-Fluoro-4'-methoxyacetophenone 18931-60-7P, 4,4,4-Trifluoro-1-[4-chlorophenyl]butane-1,3-dione 170570-77-1P, 4,4-Difluoro-1-(3-fluoro-4-methoxyphenyl)butane-1,3-dione
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 4-(1H-pyrazol-1-yl)benzenesulfonamides as antiinflammatories)

IT 60940-34-3, Ebselen 71125-38-7, Meloxicam 80937-31-1, Flosulide 110501-66-1, TMK 688 117423-95-7, LY 213024 123653-11-2, Taisho NS 398 128253-31-6, Bay-X 1005 133430-69-0, ETH 615 134578-96-4, ONO 4057 135199-82-5, LY 264086 135893-33-3, PF 10042 136326-31-3, WAY 121006 142422-79-5, RP 66153 146461-98-5, SM 15178 147398-01-4, CGS 25019C 147432-77-7, BI RM 270 150399-22-7, SB 201993 153633-01-3, SC 53228 161172-51-6, LY 293111 162011-90-7, 2(5H)-Furanone, 4-[4-(methylsulfonyl)phenyl]-3-phenyl- 180208-37-1, SB 201146
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of 4-(1H-pyrazol-1-yl)benzenesulfonamides as antiinflammatories)

RE.CNT 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Anon; EP 485111 1992 HCAPLUS
(2) Anon; WO 9404522 1994 HCAPLUS
(3) Anon; WO 9413635 1994 HCAPLUS
(4) Anon; WO 9415932 1994 HCAPLUS
(5) Anon; WO 9420480 1994 HCAPLUS
(6) Anon; WO 9426731 1994 HCAPLUS
(7) Anon; WO 9427980 1994 HCAPLUS
(8) Anon; WO 9500501 1994 HCAPLUS
(9) Anon; DE A4228201 1994
(10) Anon; WO 9603387 1996 HCAPLUS
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IT **329900-75-6, Cyclooxygenase-2**
RL: **PAC (Pharmacological activity)**; BIOL (Biological study); **THU (Therapeutic use)**
(preparation of 4-(1H-pyrazol-1-yl)benzenesulfonamides as antiinflammatories)

RN 329900-75-6 HCAPLUS
CN Synthetase, prostaglandin endoperoxide, 2 (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L102 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN **2000:277839** HCAPLUS
DN **132:313696**
ED Entered STN: 28 Apr 2000
TI Irrigation solution and method for inhibition of pain and inflammation
IN Demopulos, Gregory A.; Palmer, Pamela P.; Herz, Jeffrey M.
PA Omeros Medical Systems, Inc., USA
SO PCT Int. Appl., 114 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM A61K031-00
CC 63-6 (Pharmaceuticals)
Section cross-reference(s): 1, 2, 13
FAN.CNT 14

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000023061	A2	20000427	WO 1999-US24557	19991020
	WO 2000023061	A3	20001116		

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM,

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            AZ, BY, KG, KZ, MD, RU, TJ, TM
        RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
            DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
            CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
    AU 2000012148        A5    20000508    AU 2000-12148          19991020
    US 2002028798        A1    20020307    US 2001-839633         20010420 <--
PRAI US 1998-105166P     P     19981021
    US 1994-353775       B2    19941212  <--
    WO 1995-US16028      A2    19951212  <--
    US 1996-670699       A2    19960626
    US 1998-72913        A2    19980504
    US 1998-105026P      P     19981020
    US 1998-105029P      P     19981020
    US 1998-105044P      P     19981020
    US 1998-107256P      P     19981105
    WO 1999-US24557      W     19991020
    WO 1999-US24558      A2    19991020
    WO 1999-US24625      A2    19991020
    WO 1999-US24672      A2    19991020
    WO 1999-US26330      A2    19991105
CLASS
 PATENT NO.       CLASS  PATENT FAMILY CLASSIFICATION CODES
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 WO 2000023061    ICM    A61K031-00
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AB A method and solution for perioperatively inhibiting a variety of pain and inflammation processes at wounds from general surgical procedures including oral/dental procedures. The solution preferably includes at least 1 neuronal nicotinic acetylcholine receptor agonist and, optionally, addnl. multiple pain and inflammation inhibitory agents at dilute concentration in a physiol. carrier, such as saline or lactated Ringer's solution The solution is applied by continuous irrigation of a wound during a surgical procedure for preemptive inhibition of pain and while avoiding undesirable side effects associated with oral, i.m., s.c. or i.v. application of larger doses of the agents. One preferred solution to inhibit pain and inflammation includes a neuronal nicotinic acetylcholine receptor agonist, serotonin receptor-2 and serotonin receptor-3 antagonists, a histamine antagonist, a serotonin agonist, a **cyclooxygenase** inhibitor, neurokinin receptor-1 and neurokinin receptor-2 antagonists, a purinoceptor antagonist, an ATP-sensitive potassium channel opener, calcium channel, bradykinin receptor-1 and bradykinin receptor-2 antagonists, and a μ-opioid agonist. Thus, an irrigation solution for cardiovascular and general vascular therapeutic and diagnostic procedures consists of a serotonin receptor-2 antagonist, LY-53857 50 nM.

ST irrigation soln inhibition pain; inflammation inhibition irrigation soln; serotonin antagonist irrigation soln

IT Potassium channel
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(ATP-sensitive; irrigation solution for inhibition of pain and inflammation)

IT Purinoceptors
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(P2X, agonists; irrigation solution for inhibition of pain and inflammation)

IT Purinoceptor antagonists
(P2X; irrigation solution for inhibition of pain and inflammation)

IT Purinoceptors
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(P2Y, agonists; irrigation solution for inhibition of pain and inflammation)

IT Bradykinin receptors
Calcitonin gene-related peptide receptors
Interleukin receptors

Prostanoid receptors
Tachykinin receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(antagonists; irrigation solution for inhibition of pain and inflammation)

IT Drug delivery systems
(injections, i.v.; irrigation solution for inhibition of pain and inflammation)

IT 5-HT agonists
5-HT antagonists
Analgesics
Anti-inflammatory agents
Antihistamines
Cholinergic agonists
Opioid antagonists
Purinoceptor agonists
Purinoceptor antagonists
Thromboxane receptor antagonists
(irrigation solution for inhibition of pain and inflammation)

IT **Leukotriene antagonists**
Opioids
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(irrigation solution for inhibition of pain and inflammation)

IT Leukotriene receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(leukotriene B4, antagonists; irrigation solution for inhibition of pain and inflammation)

IT Leukotriene receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(leukotriene D4, antagonists; irrigation solution for inhibition of pain and inflammation)

IT Eicosanoids
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(receptor antagonists; irrigation solution for inhibition of pain and inflammation)

IT Drug delivery systems
(solns.; irrigation solution for inhibition of pain and inflammation)

IT Opioid receptors
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(κ-opioid, agonists; irrigation solution for inhibition of pain and inflammation)

IT Opioid receptors
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(δ-opioid, agonists; irrigation solution for inhibition of pain and inflammation)

IT Opioid receptors
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(μ-opioid, agonists; irrigation solution for inhibition of pain and inflammation)

IT **39391-18-9**
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(2, inhibitor; irrigation solution for inhibition of pain and inflammation)

IT 9001-01-8, Kallikrein 9013-93-8, Phospholipase 9029-60-1, Lipoxygenase
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(inhibitors; irrigation solution for inhibition of pain and inflammation)

IT 159125-41-4
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(ir rigation solution for inhibition of pain and inflammation)

IT 50-48-6 59-33-6, Mepyramine 146-48-5, Yohimbine 364-62-5, Metoclopramide 437-38-7, Fentanyl 2826-26-8, Tyrphostin 1 9087-70-1, Aprotinin 15307-86-5, Diclofenac 19794-93-5, Trazodone 21829-25-4,

Nifedipine 33876-97-0, SIN-1 50679-08-8, Terfenadine 51803-78-2
60634-51-7, LY 53857 63675-72-9, Nisoldipine 71125-38-7, Meloxicam
71800-37-8 74103-06-3, Ketorolac 80937-31-1, Flosulide 88149-94-4,
DuP 697 92454-60-9, FK-409 103628-46-2, Sumatriptan 113563-71-6,
(-)-Pinacidil 123653-11-2 128270-60-0, Hirulog 129623-01-4, GR 82334
133052-90-1, GF 109203X 138614-30-9, HOE 140 138680-92-9
146535-11-7, AG 1296 149017-66-3, PPADS 158205-05-1, L-745337
158959-32-1, SC-57666 **162054-19-5** 162626-99-5, FR 144420
168433-84-9, SC-58451 **169590-42-5**, Celecoxib 179382-91-3,
RS-57067 188627-80-7, Integrelin
RL: **BAC (Biological activity or effector, except adverse)**; BSU
(Biological study, unclassified); **THU (Therapeutic use)**; BIOL
(Biological study); USES (Uses)
(irrigation solution for inhibition of pain and inflammation)

IT **39391-18-9**
RL: **BAC (Biological activity or effector, except adverse)**; BIOL
(Biological study); **THU (Therapeutic use)**
(2, inhibitor; irrigation solution for inhibition of pain and
inflammation)

RN 39391-18-9 HCAPLUS
CN Synthetase, prostaglandin endoperoxide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L102 ANSWER 5 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:124064 HCAPLUS
DN 132:175822
ED Entered STN: 23 Feb 2000
TI 3,4-substituted pyrazoles for the treatment of inflammation
IN Lee, Len F.; Penning, Thomas D.; Kramer, Steven W.; **Talley, John J.**
PA **G.D. Searle** and Co., USA
SO U.S., 42 pp., Cont.-in-part of U.S. 5,486,534
CODEN: USXXAM
DT Patent
LA English
IC ICM A01N043-54
ICS C07D401-00; C07D231-02; C07D231-00
NCL 514256000
CC 1-7 (Pharmacology)
Section cross-reference(s): 28, 63

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6028072	A	20000222	US 1997-776090	19970609 <--
	US 5486534	A	19960123	US 1994-278297	19940721 <--
	WO 9603385	A1	19960208	WO 1995-US8788	19950720 <--
	W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
	RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
PRAI	US 1994-278297	A2	19940721 <--		
	WO 1995-US8788	W	19950720 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 6028072	ICM	A01N043-54
	ICS	C07D401-00; C07D231-02; C07D231-00
	NCL	514256000

OS MARPAT 132:175822

AB A class of pyrazolyl compds. (Markush included) is described for use in treating inflammation and inflammation-related disorders. Compound preparation is included.

ST pyrazole deriv prepn antiinflammatory; inflammation related disorder pyrazole deriv prepn

IT **Inflammation**
(inflammation-associated disorder; pyrazole derivative preparation for treatment of
inflammation and inflammation-related disorders)

IT **Analgesics**
Anti-inflammatory agents
Antiarthritics
Antipyretics
Drug delivery systems
(pyrazole derivative preparation for treatment of inflammation and inflammation-related disorders)

IT 87483-29-2P 165252-26-6P 175676-88-7P 175676-89-8P
175676-90-1P 175676-95-6P 175676-99-0P 175677-03-9P
175677-04-0P 175677-11-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction; pyrazole derivative preparation for treatment of inflammation and inflammation-related disorders)

IT **175677-06-2P 175677-08-4P**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(pyrazole derivative preparation for treatment of inflammation and inflammation-related disorders)

IT **175676-91-2P 175676-92-3P 175676-97-8P**
175676-98-9P 175677-01-7P 175677-02-8P
175677-05-1P 175677-07-3P 175677-09-5P
175677-10-8P 175677-12-0P 175677-13-1P
175677-14-2P
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(pyrazole derivative preparation for treatment of inflammation and inflammation-related disorders)

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259173-39-2 259187-06-9
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(pyrazole derivative preparation for treatment of inflammation and inflammation-related disorders)

IT **39391-18-9, Cyclooxygenase**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(pyrazole derivative preparation for treatment of inflammation and inflammation-related disorders)

IT **175676-93-4P** 175676-94-5P 175676-96-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(pyrazole derivative preparation for treatment of inflammation and inflammation-related disorders)

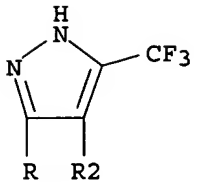
IT 62-53-3, Benzenamine, reactions 75-03-6, Ethyl iodide 100-39-0 100-68-5, Thioanisole 103-63-9, 2-Bromoethylbenzene 105-36-2, Ethyl bromoacetate 106-95-6, Allyl bromide, reactions 106-96-7, Propargyl bromide 353-85-5, Trifluoroacetonitrile 405-50-5, 4-Fluorophenylacetic acid 590-17-0, Bromoacetonitrile 1546-79-8, 1-Trifluoroacetylimidazole 4637-24-5, Dimethylformamide dimethylacetal 5050-41-9, N-(2-Chloroethyl)pyrrolidine
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction; pyrazole derivative preparation for treatment of inflammation and inflammation-related disorders)

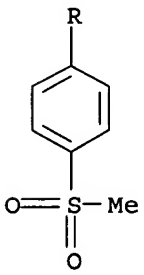
RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Adams; US 5559137 1996 HCAPLUS
(2) Isakson; US 5700816 1997 HCAPLUS

IT **175676-90-1P**
RL: **BAC (Biological activity or effector, except adverse)**; SPN (Synthetic preparation); **THU (Therapeutic use)**; **THU (Therapeutic use)**; **THU (Therapeutic use)**
(preparation and reaction; pyrazole derivative preparation for treatment of inflammation and inflammation-related disorders)

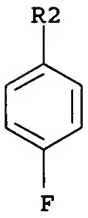
RN 175676-90-1 HCAPLUS
CN 1H-Pyrazole, 4-(4-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A





PAGE 2-A



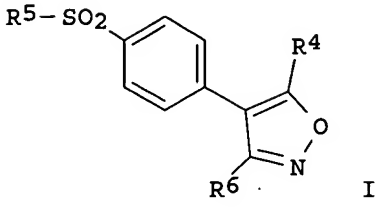
L102 ANSWER 6 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:45215 HCAPLUS
DN 130:110269
ED Entered STN: 22 Jan 1999
TI Preparation of isoxazole compounds as **cyclooxygenase** inhibitors
IN **Talley, John J.**
PA **G.D. Searle** and Co., USA
SO U.S., 52 pp., Cont.-in-part of U.S. 5,633,272.
CODEN: USXXAM
DT Patent
LA English
IC ICM C07D261-06
NCL 548247000
CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5859257	A	19990112	US 1996-702417	19960814 <--
	US 5633272	A	19970527	US 1995-473884	19950607 <--
PRAI	US 1995-387680	B2	19950213	<--	
	US 1995-473884	A2	19950607	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES

US 5859257 ICM C07D261-06
NCL 548247000
OS CASREACT 130:110269; MARPAT 130:110269
GI



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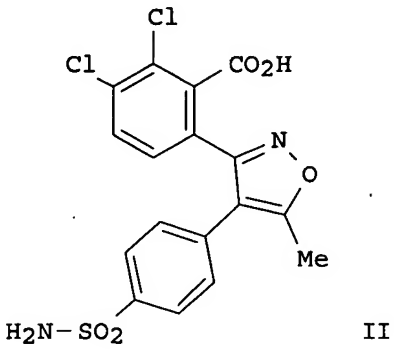

II

AB Claimed is a method of preparing title compds. I [R4 = alkyl, etc.; R5 = amino; R6 = (un)substituted phenyl] by treatment of a diphenylethanone derivative with hydroxylamine, treating said oxime with base and an acylating agent to form a diphenylisoxazoline derivative, and forming the (isoxazol-4-yl)benzenesulfonamide by treatment of the isoxazoline with chlorosulfonic acid and ammonia. The title compound II in vitro showed IC50 values of 0.4 μM and > 100 μM against **COX-2** and **COX-1**, resp.

ST isoxazole prepn **cyclooxygenase 2** inhibitor; **cyclooxygenase 2** inhibitor isoxazole prepn

IT Intestine, disease
(inflammatory; preparation and effect of isoxazole compds. with effect on **COX-2**)

IT **Analgesics**
(preparation and effect of isoxazole compds. as **cyclooxygenase** inhibitors)

IT Alzheimer's disease
Arthritis
(preparation and effect of isoxazole compds. with effect on **COX-2**)

IT **Anti-inflammatory agents**
(preparation of isoxazole compds. as **cyclooxygenase** inhibitors)

IT Intestine, disease
(ulcerative colitis; preparation and effect of isoxazole compds. with effect on **COX-2**)

IT **181695-72-7P 181695-73-8P 181695-74-9P**
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219679-65-9P
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); IMF (Industrial manufacture); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of isoxazole compds. as **cyclooxygenase** inhibitors)

IT **39391-18-9, Cyclooxygenase**
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)
(preparation of isoxazole compds. as **cyclooxygenase** inhibitors)

IT 64-17-5, Ethanol, reactions 71-43-2, Benzene, reactions 75-16-1, Methylmagnesium bromide 75-36-5, Acetyl chloride 79-20-9 98-59-9, Toluenesulfonyl chloride 99-76-3, Methyl 4-hydroxybenzoate 100-39-0, Benzyl bromide 100-52-7, Benzaldehyde, reactions 101-41-7, Methyl phenylacetate 103-79-7, Phenylacetone 103-80-0, Phenylacetyl chloride 103-82-2, Phenylacetic acid, reactions 104-87-0, p-Tolualdehyde 104-88-1, p-Chlorobenzaldehyde, reactions 108-24-7 108-30-5, Succinic anhydride, reactions 108-55-4, Glutaric anhydride 108-89-4 109-72-8, Butyllithium, reactions 110-13-4, Acetonylacetone 123-11-5, 4-Anisaldehyde, reactions 124-38-9, Carbon dioxide, reactions 321-28-8, 2-Fluoroanisole 358-23-6, Trifluoromethanesulfonic anhydride 451-40-1, Desoxybenzoin 459-57-4, 4-Fluorobenzaldehyde 553-90-2, Dimethyl oxalate 587-04-2, 3-Chlorobenzaldehyde 693-03-8, Butylmagnesium bromide 766-51-8, 2-Chloroanisole 925-90-6, Ethylmagnesium bromide 1007-32-5, 1-Phenyl-2-butanone 1122-91-4, 4-Bromobenzaldehyde 1336-21-6, Ammonium hydroxide 1722-69-6, 1,2-Diphenyl-1-buten-3-one 2466-76-4, N-Acetylimidazole 2646-90-4, 2,5-Difluorobenzaldehyde 2893-05-2 2950-43-8, Hydroxylamine O-sulfonic acid 3446-89-7, 4-(Methylthio)benzaldehyde 3795-79-7, Methyl 4-(methylthio)benzoate 4111-54-0, Lithium diisopropylamide 4166-53-4, 3-Methylglutaric anhydride 4206-67-1, Trimethylsilyliodomethane 4480-83-5, 1,4-Dioxane-2,6-dione 5188-07-8, Sodium thiomethoxide 5470-11-1, Hydroxylamine hydrochloride 6287-38-3, 3,4-Dichlorobenzaldehyde 6638-79-5, N,O-Dimethylhydroxylamine hydrochloride 6683-92-7, 1-Phenyl-2-pentanone 7446-09-5, Sulfur dioxide, reactions 7664-41-7, Ammonia, reactions 7677-24-9, Trimethylsilylcyanide 7790-94-5, Chlorosulfonic acid 13528-93-3, Bis(1,2-chlorodimethylsilyl)ethane 16188-55-9, 4-(Methylthio)phenylacetic acid 24424-99-5, Di-tert-butyl dicarbonate 34036-07-2, 3,4-Difluorobenzaldehyde 63327-11-7 88356-92-7 104372-31-8 219679-80-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of isoxazole compds. as **cyclooxygenase** inhibitors)

IT 325-62-2P 492-38-6P 952-06-7P 1023-17-2P 1529-41-5P 2001-28-7P 2001-29-8P 3475-29-4P 6318-76-9P 6574-99-8P 13721-20-5P 16736-09-7P 16736-13-3P 16737-10-3P 25632-70-6P 25870-62-6P 26306-06-9P 37612-52-5P 37928-17-9P 62482-45-5P 63954-98-3P 78967-09-6P 93534-22-6P 104896-80-2P 121411-85-6P 177560-74-6P 177561-49-8P 181696-73-1P 181696-74-2P 181696-75-3P 181696-76-4P **181696-77-5P** 181696-78-6P 181696-79-7P 181696-80-0P 181696-82-2P 181696-83-3P 181696-84-4P 181696-85-5P 181696-86-6P 181696-87-7P 181696-88-8P 181696-89-9P 181696-90-2P 181696-91-3P

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219679-79-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isoxazole compds. as **cyclooxygenase** inhibitors)

RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD

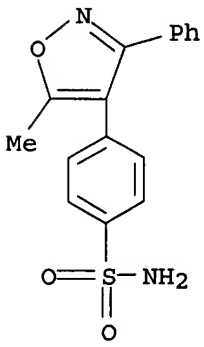
RE

(1) Anon; EP 026928 1981 HCAPLUS
(2) Anon; JP 2223568 1990
(3) Anon; JP 4173780 1992
(4) Anon; WO 9219604 1992 HCAPLUS
(5) Anon; EP 549797 1993 HCAPLUS
(6) Anon; AU 9335480 1993 HCAPLUS
(7) Anon; DE 4314966 1994 HCAPLUS
(8) Anon; EP 623603 1994 HCAPLUS
(9) Anon; WO 9417059 1994 HCAPLUS
(10) Anon; WO 9420475 1994 HCAPLUS
(11) Anon; EP 633254 1995 HCAPLUS
(12) Anon; WO 9500501 1995 HCAPLUS
(13) Anon; WO 9512587 1995 HCAPLUS
(14) Anon; WO 9514672 1995 HCAPLUS
(15) Descamps; Bull Soc Chim Belg 1964, V73, P459 HCAPLUS
(16) Hagiwara; US 5310926 1994 HCAPLUS
(17) Suzuki; US 5318970 1994 HCAPLUS
(18) Talley; US 5633272 1997 HCAPLUS
(19) Umezawa; Chem 1963, V36(9), P1150 HCAPLUS
(20) Yamawaki, I; Chem Pharm Bull 1988, V36, P3142 HCAPLUS

IT **181695-72-7P**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); IMF (Industrial manufacture); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of isoxazole compds. as **cyclooxygenase** inhibitors)

RN 181695-72-7 HCAPLUS

CN Benzenesulfonamide, 4-(5-methyl-3-phenyl-4-isoxazolyl)- (9CI) (CA INDEX NAME)



L102 ANSWER 7 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:392148 HCAPLUS
DN 129:54367
ED Entered STN: 26 Jun 1998
TI Substituted pyrazolyl benzenesulfonamides for the treatment of inflammation
IN **Talley, John J.**; Penning, Thomas D.; Collins, Paul W.; Rogier, Donald J., Jr.; Malecha, James W.; Miyashiro, Julie M.; Bertenshaw, Stephen R.; Khanna, Ish K.; **Graneto, Matthew J.**; **Rogers, Roland S.**; **Carter, Jeffery S.**; Docter, Stephen H.; Yu, Stella S.
PA **G.D. Searle** and Co., USA
SO U.S., 55 pp., Cont.-in-part of U. S. 5,521,207.
CODEN: USXXAM
DT Patent
LA English
IC ICM A61K031-415
NCL 514403000
CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5760068	A	19980602	US 1996-648113	19960906 <--
	US 5466823	A	19951114	US 1993-160594	19931130 <--
	US 5521207	A	19960528	US 1994-223629	19940406 <--
	WO 9515316	A1	19950608	WO 1994-US12720	19941114 <--
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	RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	US 6156781	A	20001205	US 1999-449076	19991124 <--
	US 6413960	B1	20020702	US 2000-609011	20000530 <--
	US 6492411	B1	20021210	US 2002-125325	20020417 <--
	US 6586603	B1	20030701	US 2002-274679	20021021 <--
	US 6716991	B1	20040406	US 2003-378781	20030304 <--
	US 2004192930	A1	20040930	US 2003-700019	20031103 <--
PRAI	US 1993-160594	A2	19931130 <--		
	US 1994-223629	A2	19940406 <--		
	WO 1994-US12720	W	19941114 <--		
	US 1996-648113	A1	19960906		
	US 1997-957345	B1	19971024		
	US 1999-449076	A1	19991124		
	US 2000-609011	A2	20000530		
	US 2002-125325	A1	20020417		
	US 2002-274679	A1	20021021		
	US 2003-378781	A1	20030304		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 5760068	ICM	A61K031-415
	NCL	514403000
US 5466823	ECLA	C07D231/12B3; C07D231/12B5; C07D231/14; C07D231/16; C07D231/54; C07D401/04; C07D405/0; C07D405/04; C07D405/04; C07D409/04; C07D409/04; <--
US 5521207	ECLA	C07D231/12B3; C07D231/12B5; C07D231/14; C07D231/16; C07D231/54; C07D401/04; C07D405/0; C07D405/04; C07D405/04; C07D409/04; C07D409/04; <--
US 6413960	ECLA	C07D231/12B3; C07D231/12B5; C07D231/14; C07D231/16; C07D231/54; C07D401/04; C07D403/0; C07D405/04;

C07D405/04; C07D405/04; C07D409/04; C07D495/04 <--
US 6492411 ECLA C07D231/12B3; C07D231/12B5; C07D231/14; C07D231/16;
C07D231/54; C07D401/04; C07D403/0; C07D405/04;
C07D405/04; C07D405/04; C07D409/04; C07D495/04 <--
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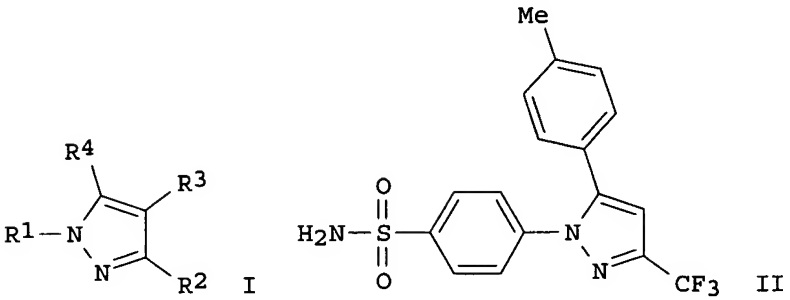
OS MARPAT 129:54367
GI



AB A class of pyrazolyl benzenesulfonamide compds. is described for use in treating inflammation and inflammation-related disorders. Several methods of such treatment are claimed, using various subsets of the title compds., e.g., I [R1 = Ph substituted by ≥1 halo, C1-10 alkyl, or sulfamyl; R2 = H, haloalkyl, alkoxycarbonyl, cyano, carboxy, aminocarbonyl, alkylaminocarbonyl, carboxyalkyl, aminocarbonylalkyl, hydroxyalkyl, etc.; R3 = H, alkyl, cyano, alkoxy, hydroxyalkyl, alkylthio, alkylsulfonyl, halo; R4 = (un)substituted aralkenyl, aryl, cycloalkyl, cycloalkenyl, heterocyclyl; with numerous provisos]. Claims also cover use of the compds. in treatment of arthritis, pain, and fever, as well as prevention of colorectal cancer. Over 260 synthetic examples are described. For instance, condensation of 4'-methylacetophenone with Et trifluoroacetate gave 94% yield of crude CF3COCH2COC6H4Me-4. This underwent cyclocondensation with 4-H2NSO2C6H4NHNH2.HCl in refluxing EtOH to give 46% yield of title compound II. The compds. typically showed high selectivity for inhibition of human **cyclooxygenase** (COX) II over COX I. Selected compds. gave 2-49% inhibition in the carrageenin-induced rat paw edema test at 10-30 mg/kg orally.

ST pyrazolylbenzenesulfonamide prepn **cyclooxygenase** inhibitor; benzenesulfonamide pyrazolyl prepn **cyclooxygenase** inhibitor; antiinflammatory pyrazolylbenzenesulfonamide prepn; analgesic pyrazolylbenzenesulfonamide prepn

IT Intestine, neoplasm
(colorectal, prevention of; preparation of pyrazolylbenzenesulfonamides as antiinflammatories)

IT Antitumor agents
(for prevention of colorectal cancer; preparation of pyrazolylbenzenesulfonamides as antiinflammatories)

IT **Analgesics**
(inhibitors of **cyclooxygenase** II; preparation of pyrazolylbenzenesulfonamides as antiinflammatories)

IT **Anti-inflammatory agents**
Antiarthritics
Antipyretics

(preparation of pyrazolylbenzenesulfonamides as antiinflammatories)

IT **39391-18-9, Cyclooxygenase**
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(inhibitors of **cyclooxygenase** II; preparation of pyrazolylbenzenesulfonamides as antiinflammatories)

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RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolylbenzenesulfonamides as antiinflammatories)

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RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolylbenzenesulfonamides as antiinflammatories)

IT 74-88-4, Methyl iodide, reactions 74-95-3, Dibromomethane 75-36-5, Acetyl chloride 77-78-1, Dimethyl sulfate 93-55-0, Propiophenone 96-48-0, γ-Butyrolactone 98-86-2, Acetophenone, reactions 99-91-2, 4'-Chloroacetophenone 100-06-1 100-58-3, Phenylmagnesium bromide 105-56-6, Ethyl cyanoacetate 106-31-0, Butyric anhydride 106-47-8, 4-Chloroaniline, reactions 108-24-7, Acetic anhydride 109-94-4, Ethyl formate 116-54-1, Methyl dichloroacetate 122-00-9, 4'-Methylacetophenone 137-06-4, o-Thiocresol 321-28-8, 2-Fluoroanisole 356-27-4, Ethyl heptafluorobutyrate 383-63-1, Ethyl trifluoroacetate 437-82-1, 2,6-Difluoroanisole 454-31-9, Ethyl difluoroacetate 488-17-5, 3-Methylcatechol 529-34-0, 1-Tetralone 553-90-2, Dimethyl oxalate 578-58-5, 2-Methylanisole 823-85-8, 4-Fluorophenylhydrazine hydrochloride 1132-05-4, 3-Allyl-4-hydroxyacetophenone 1514-87-0, Methyl chlorodifluoroacetate 1546-79-8, 1-Trifluoroacetylimidazole 1565-17-9 1984-65-2, 2,6-Dichloroanisole 2687-43-6, O-Benzylhydroxylamine hydrochloride 2746-25-0, 4-Methoxybenzyl bromide 2892-18-4, 5-Methyl-1-phenyl-1-hexen-3-one 3162-29-6 4653-11-6, 4-(2-Thienyl)butyric acid 7051-34-5, Bromomethylcyclopropane 14804-32-1, 2-Ethylanisole 22047-25-2, Acetylpyrazine 27918-19-0,

4-Sulfonamidophenylhydrazine hydrochloride 51015-29-3,
6-Methyl-1-Tetralone
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrazolylbenzenesulfonamides as antiinflammatories)

IT 318-46-7P 322-06-5P, 4,4,4-Trifluoro-2-methyl-1-phenylbutane-1,3-dione
326-06-7P, 4,4,4-Trifluoro-1-phenylbutane-1,3-dione 403-42-9P,
4'-Fluoroacetophenone 450-95-3P, 2-Fluoroacetophenone 455-91-4P
720-94-5P 2388-73-0P, 2-Methylthioanisole 6542-60-5P,
(Cyanomethyl)cyclopropane 6739-22-6P 13414-95-4P 15191-68-1P
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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrazolylbenzenesulfonamides as antiinflammatories)

RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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IT **39391-18-9, Cyclooxygenase**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); MSC (Miscellaneous); **THU (Therapeutic use)**; PROC (Process)
(inhibitors of **cyclooxygenase** II; preparation of pyrazolylbenzenesulfonamides as antiinflammatories)

RN 39391-18-9 HCAPLUS
CN Synthetase, prostaglandin endoperoxide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L102 ANSWER 8 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:146569 HCAPLUS

DN 128:192645
ED Entered STN: 11 Mar 1998
TI Preparation of [(alkylsulfonyl)phenyl]oxazoles and analogs as **cyclooxygenase** II inhibitors
IN **Norman, Bryan H.**; Lee, Len F.; Masferrer, Jaime L.; **Talley, John J.**
PA **G.D. Searle** and Co., USA
SO U.S., 51 pp., Cont.-in-part of U.S. 5,380,738.
CODEN: USXXAM
DT Patent
LA English
IC ICM C07D413-06
ICS A61K031-42; A61K031-47
NCL 514311000
CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5719163	A	19980217	US 1995-535227	19951027 <--
	US 5380738	A	19950110	US 1993-65730	19930521 <--
	WO 9427980	A1	19941208	WO 1994-US5395	19940519 <--
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	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, NL, PT, SE				
PRAI	US 1993-65730	A2	19930521 <--		
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CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 5719163	ICM	C07D413-06
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	NCL	514311000

OS MARPAT 128:192645
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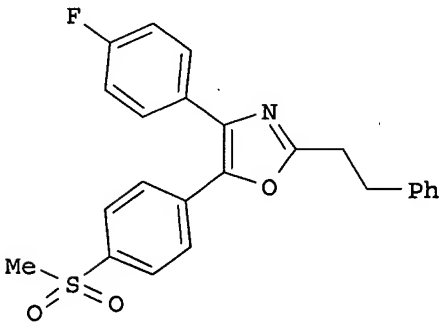

II

AB R2O2SZ2Z1R1 [I; R1 = (un)substituted cycloalk(en)yl, -(hetero)aryl; R2 = NH2 or (halo)alkyl; Z1 = 2-(un)substituted oxazolediyl; Z2 = 1,4-phenylene] were prepared Thus, 4-FC6H4COCH2C6H4(SMe)-4 was treated with NaH/Me3CMe2SiCl and the silyl enol ether product treated with 3-ClC6H4CO3H to give 4-FC6H4CH(OSiMe2CMe3)COC6H4(SMe)-4 which was deprotected and the product O-acylated by PhCH2CH2COCl to give, after cyclization, title compound II. Data for biol. activity of I were given.
ST oxazole alkylsulfonylphenyl prepn **cyclooxygenase** II inhibitor; antiinflammatory alkylsulfonylphenyloxazole prepn
IT **Analgesics**
Anti-inflammatory agents

Antiarthritics
Antipyretics
(preparation of [(alkylsulfonyl)phenyl]oxazoles and analogs as **cyclooxygenase** II inhibitors)

IT 39391-18-9
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(2; preparation of [(alkylsulfonyl)phenyl]oxazoles and analogs as **cyclooxygenase** II inhibitors)

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203518-43-8P 203518-45-0P
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of [(alkylsulfonyl)phenyl]oxazoles and analogs as **cyclooxygenase** II inhibitors)

IT **163303-50-2**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(preparation of [(alkylsulfonyl)phenyl]oxazoles and analogs as **cyclooxygenase** II inhibitors)

IT 98-88-4, Benzoyl chloride 100-39-0, Benzyl bromide 108-43-0, 3-ChloroPhenol 108-95-2, Phenol, reactions 371-41-5, 4-FluoroPhenol 405-50-5, 4-Fluorophenylacetic acid 645-45-4, Hydrocinnamoyl chloride 2043-61-0, Cyclohexanecarboxaldehyde 3446-89-7, 4-Methylthiobenzaldehyde 19810-31-2, Benzyloxyacetyl chloride 36239-09-5, Ethyl malonyl chloride 39098-75-4, 3-Cyclohexylpropionyl chloride 87483-29-2, 2-(4-Fluorophenyl)-1-(4-methylthiophenyl)ethanone 163304-91-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of [(alkylsulfonyl)phenyl]oxazoles and analogs as **cyclooxygenase** II inhibitors)

IT 36187-57-2P 71006-37-6P 157671-95-9P 163303-21-7P 163303-22-8P 163304-93-6P 163304-94-7P 163304-95-8P 163304-98-1P 163305-02-0P 163305-04-2P 163305-05-3P 163305-06-4P 185344-96-1P 185344-97-2P 185344-99-4P 203518-47-2P 203518-51-8P 203518-53-0P
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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of [(alkylsulfonyl)phenyl]oxazoles and analogs as **cyclooxygenase** II inhibitors)

RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Anon; WO 9221665 1992 HCAPLUS
(2) Anon; WO 9415932 1994 HCAPLUS
(3) Anon; WO 9427980 1994 HCAPLUS
(4) Anon; WO 9200501 1995
(5) Barreau; US 5403852 1995 HCAPLUS
(6) Brown; US 3578671 1971 HCAPLUS
(7) Carini; US 4632930 1986 HCAPLUS
(8) Cremylin, R; J Heterocycl Chem 1985, V22, P1211
(9) Dahm; US 4051250 1977 HCAPLUS
(10) Fitzi; US 3901908 1975 HCAPLUS
(11) Haber; US 4590205 1986 HCAPLUS
(12) Haber; US 4820827 1989 HCAPLUS

(13) Hafeli; US 3895024 1975 HCAPLUS
(14) Harrison; US 4143047 1979 HCAPLUS
(15) Haviv; US 4489084 1984 HCAPLUS
(16) Lutomski; US 4791124 1988 HCAPLUS
(17) Matsuo; US 5134142 1992 HCAPLUS
(18) Mattalia; US 4001228 1977 HCAPLUS
(19) Meanwell, N; J Med Chem 1992, V35, P3498 HCAPLUS
(20) Meguro; US 4775687 1988 HCAPLUS
(21) Norman; US 5380738 1995 HCAPLUS
(22) Rogers; US 4812470 1989 HCAPLUS
(23) van Es, T; J Chem Soc 1963, P1363 HCAPLUS

IT **39391-18-9**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); BIOL (Biological study); **THU (Therapeutic use)**
(2; preparation of [(alkylsulfonyl)phenyl]oxazoles and analogs as **cyclooxygenase** II inhibitors)

RN 39391-18-9 HCAPLUS
CN Synthetase, prostaglandin endoperoxide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L102 ANSWER 9 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:696748 HCAPLUS
DN 127:358861
ED Entered STN: 05 Nov 1997
TI Substituted benzenesulfonamide derivatives as prodrugs of **COX-2** inhibitors
IN **Talley, John J.**; Malecha, James W.; Bertenshaw, Stephen; **Graneto, Matthew J.**; **Carter, Jeffery S.**; Li, Jinglin; Nagarajan, Srinivasan; **Brown, David L.**; et al.
PA **G.D. Searle** and Co., USA; Talley, John J.; Malecha, James W.; Bertenshaw, Stephen; Graneto, Matthew J.; Carter, Jeffery S.; Li, Jinglin
SO PCT Int. Appl., 184 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D261-08
ICS C07D233-54; C07D401-04; A61K031-42; A61K031-415; C07D231-12; C07D495-04; C07D263-32; C07C311-39; C07D207-32; C07D307-58; C07D495-04; C07D335-00; C07D231-00
CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 25, 63
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9738986	A1	19971023	WO 1997-US5497	19970411 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
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CA 2249009	C	20030916		
AU 9727227	A1	19971107	AU 1997-27227	19970411 <--
AU 734275	B2	20010607		
EP 892791	A1	19990127	EP 1997-921092	19970411 <--
EP 892791	B1	20030305		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				

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     CN 1216043            A     19990505    CN 1997-193747          19970411 <--
     CN 1098256            B     20030108
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     JP 2000509029         T2    20000718    JP 1997-537139          19970411 <--
     JP 3382624            B2    20030304
     AP 1009               A     20010921    AP 1998-1355            19970411 <--
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     JP 2003160554         A2    20030603    JP 2002-258955          19970411 <--
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     IL 125849             A1    20031031    IL 1997-125849          19970411 <--
     ES 2194195            T3    20031116    ES 1997-921092          19970411 <--
     ZA 9703146            A     19980414    ZA 1997-3146            19970414 <--
     US 5932598            A     19990803    US 1998-5610            19980112 <--
     NO 9804727            A     19981214    NO 1998-4727            19981009 <--
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     LV 12239              B     19990820    LV 1998-215             19981012 <--
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     HK 1019741            A1    20030502    HK 1999-104900          19991101 <--
     US 6436967            B1    20020820    US 2000-661859          20000914 <--
     AU 762721             B2    20030703    AU 2001-35099           20010410
     US 2003069287         A1    20030410    US 2002-178697          20020624 <--
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     AU 1997-27227         A3    19970411
     JP 1997-537139        A3    19970411
     WO 1997-US5497        W     19970411
     EP 1997-921092        A3    19971023
     US 1999-142993        B1    19990318
     US 2000-661859        A3    20000914
CLASS
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                 ICS    C07D233-54; C07D401-04; A61K031-42; A61K031-415;
                        C07D231-12; C07D495-04; C07D263-32; C07C311-39;
                        C07D207-32; C07D307-58; C07D495-04; C07D335-00;
                        C07D231-00
 WO 9738986      ECLA   A61K031/18; A61K031/415; A61K031/415; A61K031/42;
                        A61K031/42; A61K031/635; C07C311/16; C07C; C07D207/32C;
                        C07D231/12B5; C07D233/54C3; C07D261/08; C07D263/32;
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                        C07D307/58; C07D401/04; C07D417/04; C07D495/04      <--
 US 5932598      ECLA   A61K031/18; C07D207/32C; C07D231/12B5; C07D233/54C3;
                        C07D261/08; C07D263/32; C07D307/58; C07D001/04;
                        C07D417/04; C07D495/04; A61K031/415; A61K031/415;
                        A61K031/42; A61K031/42; A61K031/635; C07C311/16;
                        C07C311/51                                          <--
 US 6436967      ECLA   A61K031/18; A61K031/415; A61K031/42; A61K031/635;
                        C07C311/16; C07D231/12B5; C07D233/54C3; C07D263/32;
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OS   MARPAT 127:358861
GI
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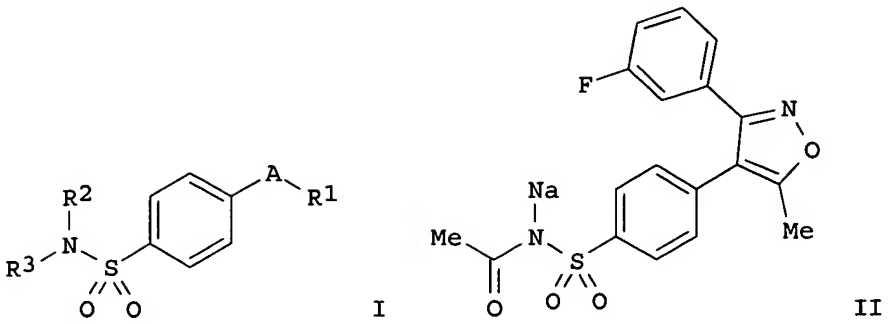

I II

AB Prodrugs of **COX-2** inhibitors, of formula I or their pharmaceutically acceptable salts, are useful in treating inflammation and inflammation-related disorders [wherein A = (un)substituted partially unsatd. heterocyclyl, heteroaryl, cycloalkenyl or aryl; R1 = (un)substituted heterocyclyl, cycloalkyl, cycloalkenyl, or aryl; R2 = H, alkoxycarbonylalkyl; R3 = alkyl, carboxyalkyl, acyl, alkoxycarbonyl, heteroarylcarbonyl, alkoxycarbonylalkylcarbonyl, alkoxycarbonylcarbonyl, amino acid residue, or alkylcarbonylaminoalkylcarbonyl; provided A ≠ tetrazolium or pyridinium, and A ≠ indanone when R3 = alkyl or carboxyalkyl]. Prepns. of over 80 compds. are described. For instance, 4-[5-methyl-3-(3-fluorophenyl)isoxazol-4-yl]benzenesulfonamide underwent N-acetylation with Ac2O, Et3N, and DMAP in THF (81%), and salification with NaOH in EtOH (97%), to give title salt II. At 30 mg/kg orally in the rat paw edema test, II gave 65% inhibition. Analgesic activity in rats, and a metabolism assay with S9 liver fractions, are also described for 3 selected compds.

ST benzenesulfonamide prepn prodrug **COX2** inhibitor; antiinflammatory analgesic benzenesulfonamide imidazole pyrazole isoxazole; **cyclooxygenase 2** inhibitor
benzenesulfonamide prodrug prepn

IT Dentistry
Neoplasm
(for treatment of pain in; preparation of substituted benzenesulfonamide derivs. as prodrugs of **COX-2** inhibitors)

IT **Analgesics**
Anti-inflammatory agents
(preparation of substituted benzenesulfonamide derivs. as prodrugs of **COX-2** inhibitors)

IT Drug delivery systems
(prodrugs; preparation of substituted benzenesulfonamide derivs. as prodrugs of **COX-2** inhibitors)

IT **39391-18-9**
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(2; preparation of substituted benzenesulfonamide derivs. as prodrugs of **COX-2** inhibitors)

IT 1709-52-0P 5635-16-5P, 3,4-Diphenyl-2(5H)-furanone 6319-45-5P 58697-03-3P 189501-41-5P 189501-42-6P 198471-84-0P 198471-85-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of substituted benzenesulfonamide derivs. as prodrugs of **COX-2** inhibitors)

IT 198471-66-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of substituted benzenesulfonamide derivs. as prodrugs of

COX-2 inhibitors)

IT 181697-32-5P 188817-04-1P 189501-10-8P 198470-65-4P 198470-66-5P
198470-67-6P 198470-69-8P 198470-71-2P 198470-72-3P 198470-73-4P
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198470-85-8P 198470-86-9P 198470-87-0P 198470-88-1P 198470-89-2P
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198471-00-0P 198471-01-1P 198471-02-2P 198471-03-3P 198471-04-4P
198471-05-5P 198471-06-6P 198471-07-7P 198471-08-8P 198471-09-9P
198471-10-2P 198471-11-3P 198471-12-4P 198471-13-5P 198471-14-6P
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198471-61-3P 198471-62-4P 198471-64-6P 198471-65-7P 198471-67-9P
198471-68-0P 198471-69-1P 198471-70-4P 198471-72-6P 198471-74-8P
198471-76-0P 198471-77-1P 198471-78-2P 198471-79-3P 198471-80-6P
198471-81-7P 198471-82-8P 198471-83-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted benzenesulfonamide derivs. as prodrugs of COX-2 inhibitors)

IT 70-11-1, Phenacyl bromide 98-74-8, 4-Nitrobenzenesulfonyl chloride
103-82-2, Phenylacetic acid, reactions 105-36-2, Ethyl bromoacetate
106-31-0, Butyric anhydride 123-62-6, Propionic anhydride 352-13-6,
4-Fluorophenylmagnesium bromide 3392-07-2 59214-95-8,
5,5-Dimethyl-1,3-dioxane-2-propanol **169590-42-5**
170569-88-7 177660-92-3 177660-94-5 177660-95-6
177661-14-2 **181695-72-7** **181696-45-7**
198471-86-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of substituted benzenesulfonamide derivs. as prodrugs of COX-2 inhibitors)

IT **39391-18-9**
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(2; preparation of substituted benzenesulfonamide derivs. as prodrugs of COX-2 inhibitors)

RN 39391-18-9 HCAPLUS
CN Synthetase, prostaglandin endoperoxide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L102 ANSWER 10 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN **1997:678926** HCAPLUS
DN **127:331392**
ED Entered STN: 25 Oct 1997
TI Preparation of 1,2-diphenylpyrroles as **cyclooxygenase-2** inhibitors
IN Kimura, Tomio; Noguchi, Yasuo; Nakao, Akira; Suzuki, Keisuke; Ushiyama, Shigeru; Kawara, Akihiro; Miyamoto, Masaaki
PA Sankyo Co., Ltd., Japan
SO Eur. Pat. Appl., 140 pp.
CODEN: EPXXDW
DT Patent
LA English
IC ICM C07D207-32
ICS A61K031-40

CC 27-10 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	EP 799823	A1	19971008	EP 1997-302245	19970402	<--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI					
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	IL 120584	A1	20031031	IL 1997-120584	19970401	<--
	AU 9716653	A1	19971009	AU 1997-16653	19970402	<--
	AU 710380	B2	19990916			
	ZA 9702846	A	19971104	ZA 1997-2846	19970403	<--
	TW 409122	B	20001021	TW 1997-86104297	19970403	<--
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CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES	
EP 799823	ICM	C07D207-32	
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US 5908858	ECLA	C07D207/32B2; C07D207/32C3	<--

OS MARPAT 127:331392
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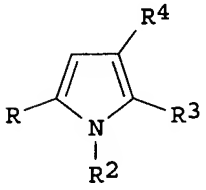

I

AB Title compds. [e.g., I; R = ZSO2R1; R1 = alkyl or NHRa; Ra = H, alkanoyl, alkoxycarbonyl, etc.; R2 = (un)substituted Ph; R3 = H, halo, (un)substituted alkyl; R4 = H, (un)substituted alkyl, aryl(alkyl), etc.; Z = (un)substituted 1,4-phenylene] were prepared Thus, 4-(MeO)C6H4NH2 was condensed with 4-(OHC)C6H4SO2Me and the product treated with Me3SiCN/ZnCl2 to give 4-(MeO)C6H4NHCH(CN)C6H4(SO2Me)-4 which was cyclocondensed with CH2:CHCHO to give I [R = C6H4(SO2Me)-4, R2 = C6H4(OMe)-4, R3 = R4 = H]. Data for biol. activity of title compds. were given.
ST phenylpyrrole prepn **cyclooxygenase 2** inhibitor
IT **Leukotrienes**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(biosynthesis inhibitors; preparation of 1,2-diphenylpyrroles as **cyclooxygenase-2** inhibitors)
IT **Analgesics**
Anti-inflammatory agents
(preparation of 1,2-diphenylpyrroles as **cyclooxygenase-2** inhibitors)
IT Bone
(resorption, inhibitors; preparation of 1,2-diphenylpyrroles as **cyclooxygenase-2** inhibitors)

IT **39391-18-9**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(2; mediated disorders; treatment; preparation of 1,2-diphenylpyrroles as **cyclooxygenase-2** inhibitors)

IT **189500-90-1P 189500-92-3P 189500-93-4P**
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RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1,2-diphenylpyrroles as **cyclooxygenase-2** inhibitors)

IT 62-53-3, Benzenamine, reactions 63-74-1, 4-Sulfamoylaniline 78-85-3, Methacrolein 78-94-4, Methyl vinyl ketone, reactions 95-64-7, 3,4-Dimethylaniline 95-76-1, 3,4-Dichloroaniline 100-52-7, Benzaldehyde, reactions 104-87-0, 4-Methylbenzaldehyde 104-88-1, 4-Chlorobenzaldehyde, reactions 104-94-9, 4-Methoxyaniline 104-96-1, 4-Methylthioaniline 105-34-0, Methyl cyanoacetate 105-45-3, Methyl acetoacetate 105-53-3, Diethyl malonate 106-47-8, 4-Chloroaniline, reactions 106-49-0, 4-Methylaniline, reactions 107-02-8, Acrolein, reactions 108-18-9, Diisopropylamine 110-89-4, Piperidine, reactions 110-96-3, Diisobutylamine 123-11-5, 4-Methoxybenzaldehyde, reactions

123-38-6, Propionaldehyde, reactions 123-72-8, Butyraldehyde 156-43-4, 4-Ethoxyaniline 351-54-2, 3-Fluoro-4-methoxybenzaldehyde 366-99-4, 3-Fluoro-4-methoxyaniline 367-21-5, 3-Chloro-4-fluoroaniline 367-25-9, 2,4-Difluoroaniline 371-40-4, 4-Fluoroaniline 372-31-6, Ethyl 4,4,4-trifluoroacetoacetate 403-29-2, 4-Fluorophenacyl bromide 455-14-1, 4-Trifluoromethylaniline 459-57-4, 4-Fluorobenzaldehyde 461-82-5, 4-Trifluoromethoxyaniline 505-57-7, 2-Hexenal 536-38-9 554-00-7, 2,4-Dichloroaniline 764-39-6, 2-Pentenal 1070-66-2, 2-Butylacrolein 1126-81-4, 4-Acetamidothiophenol 1550-35-2, 2,4-Difluorobenzaldehyde 2632-13-5, 4-Methoxyphenacyl bromide 3240-35-5, 4-Sulfamoylbenzaldehyde 3446-89-7, 4-Methylthiobenzaldehyde 3463-02-3, 4-Ethylthioaniline 3863-11-4, 3,4-Difluoroaniline 4170-30-3, Crotonaldehyde 4903-09-7, 3-Chloro-4-methoxybenzaldehyde 5398-77-6, 4-Methylsulfonylbenzaldehyde 5736-85-6, 4-Propoxybenzaldehyde 5779-95-3, 3,5-Dimethylbenzaldehyde 5973-71-7, 3,4-DimethylBenzaldehyde 6287-38-3, 3,4-Dichlorobenzaldehyde 6315-89-5, 3,4-Dimethoxyaniline 10031-82-0, 4-Ethoxybenzaldehyde 14268-66-7, 3,4-Methylenedioxyaniline 32723-67-4, 4-Methoxy-3-methylbenzaldehyde 34036-07-2, 3,4-Difluorobenzaldehyde 42445-46-5, 4-Methylthiophenacyl bromide 73960-07-3, 4-Difluoromethoxybenzaldehyde 155586-40-6, Benzamide, N-Methoxy-N,3,4-trimethyl- 175206-66-3, 3-Cyclopentyloxy-4-methoxybenzyl chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 1,2-diphenylpyrroles as **cyclooxygenase-2** inhibitors)

IT 332-15-0P 722-27-0P 3447-45-8P 5877-53-2P 39770-49-5P
64257-53-0P 64257-54-1P 66667-56-9P 69589-51-1P 87373-70-4P
100334-82-5P 105947-02-2P 106378-38-5P 109102-55-8P 112185-30-5P
189501-21-1P 197905-49-0P 197905-50-3P 197905-51-4P
197905-52-5P 197905-53-6P 197905-54-7P 197905-55-8P 197905-56-9P
197905-57-0P 197905-58-1P 197905-59-2P 197905-60-5P 197905-61-6P
197905-62-7P 197905-63-8P 197905-64-9P 197905-65-0P 197905-66-1P
197905-67-2P 197905-68-3P 197905-69-4P 197905-70-7P
197905-71-8P 197905-72-9P 197905-73-0P 197905-74-1P
197905-75-2P **197905-76-3P** 197905-77-4P **197905-78-5P**
197905-79-6P **197905-81-0P** 197905-84-3P 197905-87-6P
197905-88-7P 197905-89-8P 197905-90-1P 197905-91-2P 197905-92-3P
197905-93-4P 197905-94-5P 197905-95-6P 197905-96-7P 197905-97-8P
197905-98-9P 197905-99-0P 197906-00-6P 197906-01-7P 197906-02-8P
197906-03-9P 197906-04-0P 197906-05-1P 197906-06-2P 197906-07-3P
197906-08-4P 197906-09-5P 197906-10-8P 197906-11-9P 197906-12-0P
197906-13-1P 197906-14-2P 197906-15-3P 197906-16-4P 197906-17-5P
197906-18-6P 197906-19-7P 197906-20-0P 197906-21-1P 197906-22-2P
197906-23-3P **197906-24-4P** 197906-25-5P 197906-26-6P
197906-27-7P 197906-28-8P 197906-29-9P 197906-30-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1,2-diphenylpyrroles as **cyclooxygenase-2** inhibitors)

IT **39391-18-9**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); BIOL (Biological study); **THU (Therapeutic use)**
(2; mediated disorders; treatment; preparation of 1,2-diphenylpyrroles as **cyclooxygenase-2** inhibitors)

RN 39391-18-9 HCAPLUS
CN Synthetase, prostaglandin endoperoxide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L102 ANSWER 11 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN **1997:640654** HCAPLUS
DN **127:307375**

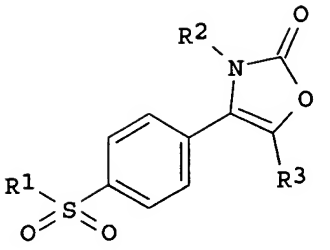
ED Entered STN: 09 Oct 1997
TI Preparation of 2-(3H)-oxazolones as **COX-2** inhibitors
IN Puig Duran, Carles; Pujol Noguera, Ferran; Fernandez Forner, Dolors
PA Grupo Farmaceutico Almirall, S.A., Spain; Puig Duran, Carles; Pujol Noguera, Ferran; Fernandez Forner, Dolores
SO PCT Int. Appl., 25 pp., none
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D263-38
ICS A61K031-42
CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	WO 9734882	A1	19970925	WO 1997-EP1386	19970319	<--
	W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
	RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
	ES 2125161	A1	19990216	ES 1996-685	19960321	<--
	ES 2125161	B1	19991116			
	ZA 9702203	A	19970925	ZA 1997-2203	19970313	<--
	CA 2249420	AA	19970925	CA 1997-2249420	19970319	<--
	AU 9722893	A1	19971010	AU 1997-22893	19970319	<--
	AU 713811	B2	19991209			
	EP 888316	A1	19990107	EP 1997-915396	19970319	<--
	EP 888316	B1	20001102			
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI					
	CN 1218459	A	19990602	CN 1997-194660	19970319	<--
	CN 1110488	B	20030604			
	BR 9708141	A	19990727	BR 1997-8141	19970319	<--
	JP 2000506876	T2	20000606	JP 1997-533156	19970319	<--
	AT 197294	E	20001115	AT 1997-915396	19970319	<--
	ES 2151254	T3	20001216	ES 1997-915396	19970319	<--
	PT 888316	T	20010228	PT 1997-915396	19970319	<--
	TW 426674	B	20010321	TW 1997-86103412	19970319	<--
	IL 126206	A1	20010614	IL 1997-126206	19970319	<--
	RU 2194043	C2	20021210	RU 1998-119076	19970319	<--
	NO 9804325	A	19981123	NO 1998-4325	19980917	<--
	HK 1015371	A1	20010713	HK 1999-100521	19990208	<--
	GR 3035096	T3	20010330	GR 2000-402784	20001218	<--
PRAI	ES 1996-685	A	19960321	<--		
	WO 1997-EP1386	W	19970319			

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 9734882	ICM	C07D263-38
	ICS	A61K031-42

OS MARPAT 127:307375
GI



I

AB The title compds. [I; R1 = alkyl, NR4R5 (wherein R4, R5 = H, alkyl, PhCH2); R2 = naphthyl, tetrahydronaphthyl, (un)substituted Ph; R3 = H, alkyl], useful in the treatment of pain, fever or inflammation, to inhibit prostanoid-induced smooth muscle contraction or for the prevention of colorectal cancer, were prepared and formulated. Thus, reaction of 4-methylsulfonylphenacyl alc. with 4-fluorophenyl isocyanate followed by refluxing the resulting 4-methylsulfonylphenacyl N-(4-fluorophenyl)carbamate in anhydrous AcOH afforded I [R1 = Me; R2 = 4-FC6H4; R3 = H] which showed IC50 of 3.2 μM against **COX-2** vs. IC50 of 127 μM against **COX-1**.

ST oxazolone prepn formulation **cyclooxygenase** inhibitor; analgesic oxazolone prepn formulation; antipyretic oxazolone prepn formulation; antiinflammatory oxazolone prepn formulation; smooth muscle contraction oxazolone prepn formulation; colorectal cancer oxazolone prepn formulation; antitumor agent oxazolone prepn formulation

IT Intestine, neoplasm
(colorectal, prevention of; preparation of 2-(3H)-oxazolones as **COX-2** inhibitors)

IT **Analgesics**
Anti-inflammatory agents
Antipyretics
Antitumor agents
(preparation of 2-(3H)-oxazolones as **COX-2** inhibitors)

IT Muscle
(smooth, prostanoid-induced smooth muscle contraction; preparation of 2-(3H)-oxazolones as **COX-2** inhibitors)

IT **39391-18-9**
RL: CAT (Catalyst use); USES (Uses)
(**cyclooxygenase-2** inhibitors; preparation of 2-(3H)-oxazolones as **COX-2** inhibitors)

IT **197239-92-2P 197239-93-3P 197239-94-4P**
197239-95-5P 197239-96-6P 197239-97-7P
197239-98-8P 197239-99-9P 197240-00-9P
197240-01-0P 197240-02-1P 197240-03-2P
197240-04-3P 197240-05-4P 197240-06-5P
197240-07-6P 197240-08-7P 197240-09-8P
197240-10-1P 197240-11-2P 197240-12-3P
197240-13-4P 197240-14-5P 197240-15-6P
197240-16-7P 197240-17-8P 197240-18-9P
197240-19-0P 197240-20-3P 197240-21-4P
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2-(3H)-oxazolones as **COX-2** inhibitors)

IT 1195-45-5, 4-Fluorophenyl isocyanate 2493-02-9, 4-Bromophenyl isocyanate 197240-27-0 197240-28-1 197240-29-2 197240-30-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 2-(3H)-oxazolones as **COX-2** inhibitors)

IT 197240-22-5P 197240-23-6P 197240-24-7P 197240-25-8P 197240-26-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2-(3H)-oxazolones as **COX-2** inhibitors)
IT **39391-18-9**
RL: **BAC (Biological activity or effector, except adverse)**; USES (Uses); **THU (Therapeutic use)**
(**cyclooxygenase-2** inhibitors; preparation of 2-(3H)-oxazolones as **COX-2** inhibitors)
RN 39391-18-9 HCAPLUS
CN Synthetase, prostaglandin endoperoxide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L102 ANSWER 12 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:562996 HCAPLUS
DN 127:239123
ED Entered STN: 04 Sep 1997
TI Combinations having immunosuppressive effects, containing **cyclooxygenase-2**-inhibitors and **5-lipoxygenase** inhibitors
IN Gregory, Susan A.; Isakson, Peter C.; Anderson, Gary
PA **G.D. Searle** and Co., USA; Gregory, Susan A.; Isakson, Peter C.; Anderson, Gary
SO PCT Int. Appl., 68 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM A61K045-06
CC 63-6 (Pharmaceuticals)
Section cross-reference(s): 1, 15
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9729776	A1	19970821	WO 1997-US1558	19970212 <--
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	CA 2246265	AA	19970821	CA 1997-2246265	19970212 <--
	AU 9718505	A1	19970902	AU 1997-18505	19970212 <--
	EP 888127	A1	19990107	EP 1997-904133	19970212 <--
	EP 888127	B1	20011212		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
	JP 2000504723	T2	20000418	JP 1997-529363	19970212 <--
	AT 210461	E	20011215	AT 1997-904133	19970212 <--
	PT 888127	T	20020531	PT 1997-904133	19970212 <--
	ES 2169351	T3	20020701	ES 1997-904133	19970212 <--
	US 6376528	B1	20020423	US 1999-430072	19991018 <--
	US 2002143033	A1	20021003	US 2002-98644	20020315 <--
PRAI	US 1996-600622	A1	19960213	<--	
	WO 1997-US1558	W	19970212		
	US 1998-189463	B1	19981110		
	US 1999-430072	A3	19991018		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 9729776	ICM	A61K045-06
US 2002143033	ECLA	A61K045/06; H01M002/26; H01M004/24; H01M004/26 <--

OS MARPAT 127:239123

AB Treatment with a **cyclooxygenase-2** inhibitor and a **5-lipoxygenase** inhibitor is described as being useful in reducing recipient rejection of transplanted organs and for treatment of autoimmune diseases. 4-[5-(3-Fluoro-4-methoxyphenyl)-3-(difluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide and N'-[3-[5-(4-fluorophenoxy)-2-furyl]-1-methyl-2-propynyl]-N'-hydroxyurea were prepared and a combination of these 2 compds. showed a delay in rejection time of skin grafts while treatment alone of each of these compds. resulted in no prolongation of graft survival.

ST **cyclooxygenase** lipoxygenase inhibitor immunosuppressant

IT Autoimmune disease
Immunosuppressants
Inflammation
Transplant and Transplantation
(**cyclooxygenase-2** and **5-lipoxygenase** inhibitor combinations with immunosuppressive effects)

IT **39391-18-9**
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(2-, inhibitors; **cyclooxygenase-2** and **5-lipoxygenase** inhibitor combinations with immunosuppressive effects)

IT 134470-38-5, BW-B 70C
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(BW-B 70C; **cyclooxygenase-2** and **5-lipoxygenase** inhibitor combinations with immunosuppressive effects)

IT 187112-47-6, R 840
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(R 840; **cyclooxygenase-2** and **5-lipoxygenase** inhibitor combinations with immunosuppressive effects)

IT 141579-67-1P, A-78773 **169590-41-4P 170569-86-5P**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(**cyclooxygenase-2** and **5-lipoxygenase** inhibitor combinations with immunosuppressive effects)

IT 99-91-2, 4'-Chloroacetophenone 321-28-8, 2-Fluoroanisole 383-63-1, Ethyl trifluoroacetate 454-31-9, Ethyl difluoroacetate 27918-19-0, 4-Sulfonamidophenylhydrazine hydrochloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(**cyclooxygenase-2** and **5-lipoxygenase** inhibitor combinations with immunosuppressive effects)

IT 455-91-4P, 3'-Fluoro-4'-methoxyacetophenone 18931-60-7P 170570-77-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(**cyclooxygenase-2** and **5-lipoxygenase** inhibitor combinations with immunosuppressive effects)

IT 341-88-8, KF-8940 4737-26-2, Isoflavan 27686-84-6, Masoprocol 34334-69-5, Cirsiliol 36441-32-4, DuP-654 46721-85-1, CBS-1114 60284-71-1, AHR-5333 71125-38-7, Meloxicam 75139-38-7, Carbazomycin B 79916-77-1, Forsythiaside 80809-81-0, Docebenone 80937-31-1, Flosulide 87660-25-1, ONO 5349 88149-94-4, Dup 697 91431-42-4, Lonapalene 92532-05-3, Rev 5367 **93014-16-5** 93211-49-5, L-651392 96314-49-7, TEI-8005 96920-48-8, TMK 992 96928-53-9, TMK-919 99107-52-5, Bunaprolast 99134-29-9, L-651896 99318-09-9, QA-208-199 100035-75-4, Evandamine 101335-99-3, Eprovafen 101618-31-9, TMK 789 101619-08-3, TMK 781 101619-11-8, TMK-777 101910-24-1, PF-5901

102612-16-8, L-656224 103141-09-9, FPL 62064 103475-41-8, Tepoxalin
104007-80-9, TZI-41127 104153-37-9, Rilopirox 105357-17-3, SC-41661A
107008-29-7, L-652343 107746-52-1, E 5110 107889-32-7, LY-178002
110033-17-5, WY 47288 110406-33-2 110545-79-4, SCH 40120
111406-87-2, Zileuton 111525-11-2, A-63162 111908-94-2, SK&F-104351
111908-95-3, SK&F-104493 111974-60-8, WY-48252 112344-52-2, Flobufen
114832-13-2, CGS 8515 114917-95-2, BMY-30094 115255-10-2, ONO-LP 219
115255-23-7, ONO-LP 269 115816-05-2, BI-L-93BS 117574-40-0, CV-6504
118414-82-7, MK-886 118420-47-6, Tagorizine 119256-94-9, FR 110302
120164-49-0, E-6080 120210-48-2, Tenidap 120602-97-3, RG-6866
121135-51-1 121412-39-3, CGS-21595 121502-05-4, PD-127443
122454-69-7, SK&F-105809 122610-85-9, A-65260 123016-21-7, WY-50295
123606-23-5, A-69412 123653-11-2, NS-398 125721-82-6, BIL 226XX
125722-16-9, Enofelast 127245-22-1, BF-389 127378-46-5, CI 987
127481-38-3, L-674636 128253-31-6, BAY-X-1005 129424-08-4, ICI-211965
130116-16-4, CI-986 130211-54-0, T-799 130211-75-5, T-757
130838-15-2, Y-19432 131817-86-2, CGS 22745 132392-65-5, LY-269415
132734-43-1, LY-233569 132956-22-0, Enazadrem phosphate 133174-26-2,
L-670630 133430-69-0, ETH-615 134470-36-3, BW-B 218C 134822-78-9,
CGS-23885 134823-10-2, CGS 24891 135133-84-5, SC-45662 135872-69-4,
WAY 120739 135872-94-5, WAY 121520 138331-04-1, R-68151 139149-55-6,
SB-202235 139340-56-0, CI-1004 140841-32-3, ZD02138 141579-54-6, A
76745 141579-87-5, A-79175 143964-80-1, F-1322 145096-30-6, E 3040
146935-39-9, Epocarbazolin A 147030-01-1, MK-591 147317-96-2,
Nitrosoxacin A 147497-10-7, CGS 26529 147936-06-9, L 699333
148915-76-8, BU 4601A 149539-02-6, BI-L-357 150693-65-5, Lagunamycin
153950-29-9, A 121798 154214-70-7, R-85355 154355-76-7, ABT 761
155944-23-3, ZM-230487 156897-06-2, ML-3000 158930-07-5, L 739010
162011-90-7 177660-77-4 177660-80-9 177660-92-3 **181695-72-7**
185344-51-8 185344-55-2 187112-03-4, A 72694
187112-04-5, A-80263 187112-09-0, Bay-q-1531 187112-10-3, BF-397
187112-11-4, BW 4C 187112-12-5, BW-70C 187112-17-0, CHF-1909
187112-22-7, EF-40 187112-23-8, EN-105 187112-26-1, FPL-64170
187112-28-3, GR-80907 187112-30-7, HX 0386 187112-32-9, L-691816
187112-33-0, Linazolast 187112-35-2, LY-280810 187112-36-3, MM-7002
187112-41-0, P 8892 187112-42-1, P 8977 187112-43-2, PD-136005
187112-44-3, PD-145246 187112-50-1, RU-46057 187112-52-3, SL-81-0433
187112-54-5, SS 81OH 187112-58-9, TMK 685 187112-59-0, TZI-2721
187112-62-5, WAY-125007 187112-64-7, ZD 7717 187112-65-8, ZM-216800
193739-23-0, CMI-392 **195061-34-8** 195065-56-6
195065-57-7 195215-27-1, Carbazoycin C 195215-52-2, RG 5901A
RL: **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(**cyclooxygenase-2** and **5-lipoxygenase** inhibitor combinations with immunosuppressive effects)

IT **80619-02-9, 5-Lipoxygenase**
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(inhibitors; **cyclooxygenase-2** and **5-lipoxygenase** inhibitor combinations with immunosuppressive effects)

IT **39391-18-9**
RL: **THU (Therapeutic use)**; BIOL (Biological study); **THU (Therapeutic use)**
(2-, inhibitors; **cyclooxygenase-2** and **5-lipoxygenase** inhibitor combinations with immunosuppressive effects)

RN 39391-18-9 HCAPLUS
CN Synthetase, prostaglandin endoperoxide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L102 ANSWER 13 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:557660 HCAPLUS

DN 127:239120
ED Entered STN: 01 Sep 1997
TI Compositions comprising a **cyclooxygenase-2** inhibitor and a leukotriene B4 receptor antagonist for reducing transplant rejection
IN Gregory, Susan A.; Isakson, Peter C.; Anderson, Gary
PA **G.D. Searle** and Co., USA; Gregory, Susan A.; Isakson, Peter C.; Anderson, Gary
SO PCT Int. Appl., 63 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM A61K045-06
ICS A61K031-00; A61K031-10; A61K031-18; A61K038-13
CC 63-6 (Pharmaceuticals)
Section cross-reference(s): 1, 2
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	WO 9729775	A1	19970821	WO 1997-US1422	19970211	<--
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
	CA 2246356	AA	19970821	CA 1997-2246356	19970211	<--
	AU 9722500	A1	19970902	AU 1997-22500	19970211	<--
	EP 880362	A1	19981202	EP 1997-905663	19970211	<--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI					
	JP 2000505445	T2	20000509	JP 1997-529359	19970211	<--
	US 6172096	B1	20010109	US 1998-75633	19980511	<--
	US 6617345	B1	20030909	US 2000-659299	20000912	<--
	US 2004106668	A1	20040603	US 2003-617222	20030710	<--
PRAI	US 1996-600580	A1	19960213	<--		
	WO 1997-US1422	W	19970211			
	US 1998-75633	A3	19980511			
	US 2000-659299	A3	20000912			

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES	
WO 9729775	ICM	A61K045-06	
	ICS	A61K031-00; A61K031-10; A61K031-18; A61K038-13	
US 6617345	ECLA	A61K038/13; A61K045/06	<--
US 2004106668	ECLA	A61K038/13; A61K045/06	<--

OS MARPAT 127:239120
AB Treatment with a **cyclooxygenase-2** inhibitor and a leukotriene B4 receptor antagonist is described as being useful in reducing recipient rejection of transplanted organs and for treatment of autoimmune diseases.
ST immunodepressant transplant cyclooxygenase2 inhibitor leukotrieneB4 antagonist
IT Kidney, disease
(Goodpasture's syndrome; compns. comprising a **cyclooxygenase-2** inhibitor and a leukotriene B4 receptor antagonist for reducing transplant rejection)
IT Leukocyte
(activation of, inhibitors of; compns. comprising a **cyclooxygenase-2** inhibitor and a leukotriene B4 receptor antagonist for reducing transplant rejection)
IT **Anti-inflammatory agents**
Autoimmune disease

Encephalomyelitis
Granuloma
Immunosuppressants
Meningitis
Urticaria
(compns. comprising a **cyclooxygenase-2** inhibitor and a leukotriene B4 receptor antagonist for reducing transplant rejection)

IT Myasthenia gravis
Sjogren's syndrome
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(compns. comprising a **cyclooxygenase-2** inhibitor and a leukotriene B4 receptor antagonist for reducing transplant rejection)

IT **Dermatitis**
(contact; compns. comprising a **cyclooxygenase-2** inhibitor and a leukotriene B4 receptor antagonist for reducing transplant rejection)

IT Drug delivery systems
(emulsions; compns. comprising a **cyclooxygenase-2** inhibitor and a leukotriene B4 receptor antagonist for reducing transplant rejection)

IT Kidney, disease
(glomerulonephritis; compns. comprising a **cyclooxygenase-2** inhibitor and a leukotriene B4 receptor antagonist for reducing transplant rejection)

IT Transplant and Transplantation
(graft-vs.-host reaction; compns. comprising a **cyclooxygenase-2** inhibitor and a leukotriene B4 receptor antagonist for reducing transplant rejection)

IT Anemia (disease)
(hemolytic; compns. comprising a **cyclooxygenase-2** inhibitor and a leukotriene B4 receptor antagonist for reducing transplant rejection)

IT Lung, disease
(hypersensitivity pneumonitis; compns. comprising a **cyclooxygenase-2** inhibitor and a leukotriene B4 receptor antagonist for reducing transplant rejection)

IT Addison's disease
(idiopathic; compns. comprising a **cyclooxygenase-2** inhibitor and a leukotriene B4 receptor antagonist for reducing transplant rejection)

IT Leukotriene receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(leukotriene B4, antagonists; compns. comprising a **cyclooxygenase-2** inhibitor and a leukotriene B4 receptor antagonist for reducing transplant rejection)

IT Drug delivery systems
(oral; compns. comprising a **cyclooxygenase-2** inhibitor and a leukotriene B4 receptor antagonist for reducing transplant rejection)

IT Shock (circulatory collapse)
(septic; compns. comprising a **cyclooxygenase-2** inhibitor and a leukotriene B4 receptor antagonist for reducing transplant rejection)

IT Purpura (disease)
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(thrombocytopenic, autoimmune; compns. comprising a **cyclooxygenase-2** inhibitor and a leukotriene B4

receptor antagonist for reducing transplant rejection)
IT Thyroid gland, disease
Thyroid gland, disease
(thyroiditis; compns. comprising a **cyclooxygenase-2** inhibitor and a leukotriene B4 receptor antagonist for reducing transplant rejection)
IT **39391-18-9**
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(2, antagonists; compns. comprising a **cyclooxygenase-2** inhibitor and a leukotriene B4 receptor antagonist for reducing transplant rejection)
IT 127378-46-5, CI 987
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(CI 987; compns. comprising a **cyclooxygenase-2** inhibitor and a leukotriene B4 receptor antagonist for reducing transplant rejection)
IT **170569-86-5P** 195061-35-9P
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(compns. comprising a **cyclooxygenase-2** inhibitor and a leukotriene B4 receptor antagonist for reducing transplant rejection)
IT 32222-06-3, Calcitriol 59865-13-3, Cyclosporin a 60940-34-3, Ebselen
71125-38-7, Meloxicam 79217-60-0, Cyclosporin 80937-31-1, Flosulide
85259-71-8, BAY 0-8276 88149-94-4, Dup 697 **93014-16-5**
101910-24-1, PF-5901 110501-66-1, TMK-688 111908-95-3, SK&F-104493
117423-74-2, LY 223982 117423-95-7, LY 213024 117690-79-6, LY-255283
118414-82-7, MK-886 119261-58-4, TEI 1338 120072-59-5, SC-41930
123653-11-2, NS-398 128253-31-6, Bay-x-1005 130211-75-5, T-757
132734-43-1, LY 233569 133430-69-0, ETH-615 134578-96-4, ONO LB457
135199-82-5, LY 264086 135893-33-3, PF 10042 136326-31-3, WAY 121006
141059-52-1, SC-51146 141748-00-7, RP 69698 141835-49-6, RG 14893
142422-79-5, RP 66153 146461-98-5, SM 15178 147030-01-1, MK-591
147398-01-4, CGS-25019C 147432-77-7, Ontazolast 150399-22-7, SB-201993
153034-77-6, LY 292728 153633-01-3, SC-53228 154413-61-3, SB-209247
158081-99-3, Pfizer 105696 158089-95-3, S 2474 161172-51-6, LY-293111
162011-83-8 162011-90-7 162153-46-0, SC 52798 **169590-41-4**
169590-42-5 177660-77-4 177660-80-9 177660-92-3
180208-37-1, SB-201146 **181695-72-7 185344-51-8**
185344-55-2 186912-85-6, ONO-LB-448 186912-92-5, RP 66364
186912-94-7, SC-50505 **195061-34-8** 195215-25-9, BPC 15
195215-47-5, MNX 160 195215-55-5, SR 2566
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(compns. comprising a **cyclooxygenase-2** inhibitor and a leukotriene B4 receptor antagonist for reducing transplant rejection)
IT 99-91-2, 4'-Chloroacetophenone 383-63-1, Ethyl trifluoroacetate
454-31-9, Ethyl difluoroacetate 27918-19-0, 4-Sulfonamidophenyl hydrazine hydrochloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(compns. comprising a **cyclooxygenase-2** inhibitor and a leukotriene B4 receptor antagonist for reducing transplant rejection)
IT 455-91-4P, 3'-Fluoro-4'-methoxyacetophenone 18931-60-7P 170570-77-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(compns. comprising a **cyclooxygenase-2** inhibitor

and a leukotriene B4 receptor antagonist for reducing transplant rejection)

IT **39391-18-9**
RL: **BAC (Biological activity or effector, except adverse)**; BIOL (Biological study); **THU (Therapeutic use)**; **THU (Therapeutic use)**
(2, antagonists; compns. comprising a **cyclooxygenase-2** inhibitor and a leukotriene B4 receptor antagonist for reducing transplant rejection)

RN 39391-18-9 HCAPLUS
CN Synthetase, prostaglandin endoperoxide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L102 ANSWER 14 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:411072 HCAPLUS
DN 127:108929
ED Entered STN: 03 Jul 1997
TI Preparation of 1,4,5-triphenylpyrazoles for the treatment of inflammation and inflammation-related disorders
IN Lee, Len F.
PA **G.D. Searle** and Co., USA
SO U.S., 18 pp., Cont.-in-part of U.S. 5,401,765.
CODEN: USXXAM
DT Patent
LA English
IC ICM A61K031-415
ICS C07D231-12; C07D231-14
NCL 514406000
CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5639777	A	19970617	US 1996-648118	19960521 <--
	US 5401765	A	19950328	US 1993-161004	19931130 <--
	WO 9515317	A1	19950608	WO 1994-US12721	19941114 <--

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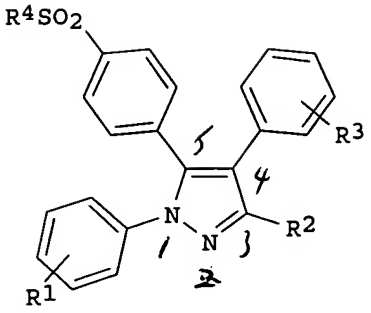
RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

PRAI US 1993-161004 19931130 <--
WO 1994-US12721 19941114 <--

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 5639777	ICM	A61K031-415
	ICS	C07D231-12; C07D231-14
	NCL	514406000

OS MARPAT 127:108929
GI



I

AB The title compds. [I; R1 = H, halo, C1-20 alkyl, etc.; R2 = H, C1-20 alkyl, CN, C1-20 haloalkyl; R3 = H, halo, C1-20 alkyl, etc.; R4 = NH2], useful for the treatment of inflammation, including treatment of pain and disorders such as arthritis, were prepared Thus, treatment of 2-(4-fluorophenyl)-1-[4-(methylthio)phenyl]ethanone with NaH in DMF followed by passing of gaseous CF3CN to the above mixture, treatment of the resulting 3-amino-4,4,4-trifluoro-2-(4-fluorophenyl)-1-[4-(methylthio)phenyl]-2-buten-1-one with 6N HCl, reaction of 2-(4-fluorophenyl)-1-[4-(methylthio)phenyl]-4,4,4-trifluoro-1,3-butanedione with PhNHNH2 in AcOH, and treatment of 4-(4-fluorophenyl)-5-[4-(methylthio)phenyl]-1-phenyl-3-(trifluoromethyl)pyrazole with 30% H2O2 in AcOH afforded I [R1 = H; R2 = CF3; R3 = 4-F; R4 = Me] which showed 20% rat paw edema inhibition at 10 mg/kg body weight

ST phenylpyrazole prepn antiinflammatory analgesic antiarthritic

IT **Analgesics**
Anti-inflammatory agents
Antiarthritics
(preparation of 1,4,5-triphenylpyrazoles for the treatment of inflammation and inflammation-related disorders)

IT **165251-89-8P 192449-77-7P 192449-78-8P**
192449-79-9P 192449-80-2P 192449-81-3P
192449-82-4P 192449-83-5P 192449-84-6P
192449-85-7P 192449-86-8P 192449-87-9P
192449-88-0P 192449-89-1P 192449-90-4P
192449-91-5P 192449-92-6P 192449-93-7P
192449-94-8P 192449-95-9P 192449-96-0P
192449-97-1P 192449-98-2P 192449-99-3P
192450-00-3P 192450-01-4P 192450-02-5P
192450-03-6P 192450-04-7P 192450-05-8P
192450-06-9P 192450-07-0P 192450-08-1P
192450-09-2P 192450-10-5P 192450-11-6P
192450-12-7P 192450-13-8P
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1,4,5-triphenylpyrazoles for the treatment of inflammation and inflammation-related disorders)

IT 165252-29-9P
RL: BYP (Byproduct); PREP (Preparation)
(preparation of 1,4,5-triphenylpyrazoles for the treatment of inflammation and inflammation-related disorders)

IT 100-63-0, Phenylhydrazine 87483-29-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 1,4,5-triphenylpyrazoles for the treatment of inflammation and inflammation-related disorders)

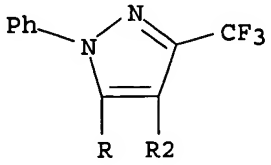
IT 165252-26-6P 165252-27-7P 165252-28-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

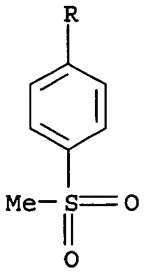
(Reactant or reagent)
(preparation of 1,4,5-triphenylpyrazoles for the treatment of inflammation and inflammation-related disorders)

IT **165251-89-8P**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1,4,5-triphenylpyrazoles for the treatment of inflammation and inflammation-related disorders)

RN 165251-89-8 HCAPLUS
CN 1H-Pyrazole, 4-(4-fluorophenyl)-5-[4-(methylsulfonyl)phenyl]-1-phenyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A





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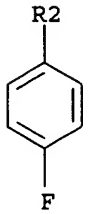

L102 ANSWER 15 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:380997 HCAPLUS
DN 126:343566
ED Entered STN: 19 Jun 1997
TI Method of detecting **cyclooxygenase-2** using pyrazolylbenzenesulfonamide imaging agents
IN Isakson, Peter C.; Seibert, Karen; **Talley, John J.**
PA **G.D. Searle** and Co., USA; Isakson, Peter C.; Seibert, Karen; Talley, John J.
SO PCT Int. Appl., 62 pp.
CODEN: PIXXD2
DT Patent

LA English
IC ICM C07D
CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9714679	A2	19970424	WO 1996-US16440	19961016 <--
	WO 9714679	A3	19970814		
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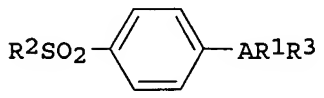
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM				
	CA 2234633	AA	19970424	CA 1996-2234633	19961016 <--
	AU 9676629	A1	19970507	AU 1996-76629	19961016 <--
	AU 716582	B2	20000302		
	EP 859642	A2	19980826	EP 1996-939457	19961016 <--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
	BR 9611047	A	20000308	BR 1996-11047	19961016 <--
	JP 2000510816	T2	20000822	JP 1997-515911	19961016 <--
	NO 9801708	A	19980610	NO 1998-1708	19980416 <--
	US 6045773	A	20000404	US 1999-256739	19990224 <--
	US 2001055565	A1	20011227	US 2001-756893	20010109 <--
PRAI	US 1995-5686P	P	19951017 <--		
	US 1996-731618	B1	19961016		
	WO 1996-US16440	W	19961016		
	US 2000-506064	B1	20000217		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 9714679	ICM	C07D

OS MARPAT 126:343566
GI



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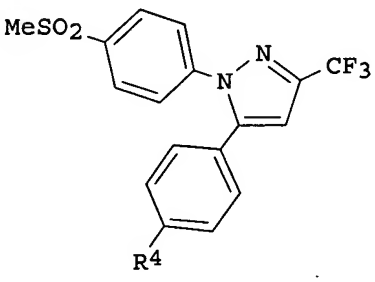


II

AB A method of detecting concns. of **cyclooxygenase-2** in a mammal comprises: (a) administering to the mammal a diagnostically effective amount of a **cyclooxygenase-2** selective agents, e.g pyrazolylbenzenesulfonamides I [A = partially unsatd. heterocyclyl, heteroaryl, cycloalkenyl, aryl; R1 = substituted heteroaryl, cycloalkyl, cycloalkenyl; R2 = Me, NH2; R3 = H, halo, oxo, CN, amino, (un)substituted

alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, heterocyclyl, aryl, acyl, alkoxycarbonyl, aminocarbonyl, alkoxy, aryloxy, alkylthio, arylthio, alkylsulfinyl, alkylsulfonyl, aminosulfonyl, arylsulfonyl], which are capable of being detected in vivo; and (b) detecting the agent so the concentration of **cyclooxygenase-2** is determined Isotopically labeled I (R1 contains isotopically labeled substituent, e.g. 11C, 123I, 73Se, 76Br, 77Br, 18F), capable of being detected in vivo by PET, are also claimed. Thus, pyrazole II (R4 = 18F) was prepared from 4-MeSO2C6H4NHNH2.HCl and 4-O2NC6H4COCH2COCF3 via nucleophilic substitution of II (R4 = NO2) with an 18F source.

ST pyrazolylbenzenesulfonamide radiolabeled imaging agent prepn; **cyclooxygenase 2** inhibitor radiolabeled pyrazolylbenzenesulfonamide prepn; PET contrast agent radiolabeled pyrazolylbenzenesulfonamide prepn

IT Tomography
Tomography
(contrast agents; detection of **cyclooxygenase-2** using pyrazolylbenzenesulfonamide PET imaging agents)

IT Imaging agents
Imaging agents
(contrast, tomog.; detection of **cyclooxygenase-2** using pyrazolylbenzenesulfonamide PET imaging agents)

IT Positron-emission tomography
(detection of **cyclooxygenase-2** using pyrazolylbenzenesulfonamide PET imaging agents)

IT **39391-18-9**, **Cyclooxygenase**
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(2; detection of **cyclooxygenase-2** using pyrazolylbenzenesulfonamide PET imaging agents)

IT 100-19-6 383-63-1, Ethyl trifluoroacetate 454-31-9, Ethyl difluoroacetate 553-90-2, Dimethyl oxalate 582-65-0 17852-67-4, 4-(Methylsulfonyl)phenylhydrazine hydrochloride 27918-19-0, 4-(Sulfonamido)phenylhydrazine hydrochloride 54696-05-8, 4-(Benzyloxy)acetophenone
RL: RCT (Reactant); RACT (Reactant or reagent)
(detection of **cyclooxygenase-2** using pyrazolylbenzenesulfonamide PET imaging agents)

IT 35999-53-2P **151507-18-5P** **190020-10-1P** **190020-11-2P** 190020-12-3P **190020-13-4P** 190020-14-5P **190020-15-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(detection of **cyclooxygenase-2** using pyrazolylbenzenesulfonamide PET imaging agents)

IT **170571-05-8P** **188816-86-6P** **190019-66-0P** **190019-67-1P** **190019-68-2P** 190019-69-3P 190019-70-6P **190019-71-7P** **190019-72-8P** **190019-73-9P** **190019-74-0P** **190019-75-1P** **190019-76-2P** **190019-77-3P** **190019-78-4P** 190019-79-5P 190019-80-8P **190019-81-9P** **190019-82-0P** **190019-83-1P** **190019-84-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(detection of **cyclooxygenase-2** using pyrazolylbenzenesulfonamide PET imaging agents)

IT **162054-19-5P** **170569-88-7P** **190019-85-3P** **190019-86-4P** **190019-87-5P** **190019-88-6P** 190019-89-7P 190019-90-0P **190019-91-1P** **190019-92-2P** **190019-93-3P** **190019-94-4P** **190019-95-5P** **190019-96-6P** **190019-97-7P** **190019-98-8P** **190019-99-9P** 190020-00-9P 190020-01-0P **190020-02-1P** **190020-03-2P** **190020-04-3P** **190020-05-4P**

190020-06-5P 190020-07-6P 190020-08-7P
190020-09-8P
RL: SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(detection of **cyclooxygenase-2** using pyrazolylbenzenesulfonamide PET imaging agents)

IT **39391-18-9, Cyclooxygenase**
RL: BSU (Biological study, unclassified); **THU (Therapeutic use)**; **THU (Therapeutic use)**
(2; detection of **cyclooxygenase-2** using pyrazolylbenzenesulfonamide PET imaging agents)

RN 39391-18-9 HCAPLUS
CN Synthetase, prostaglandin endoperoxide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L102 ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:372654 HCAPLUS
DN 127:65756
ED Entered STN: 14 Jun 1997
TI Preparation of substituted isoxazoles for the treatment of inflammation
IN **Talley, John J.**; **Brown, David L.**; Nagarajan, Srinivasan; **Carter, Jeffery S.**; Weier, Richard M.; Stealey, Michael A.; Collins, Paul W.; **Rogers, Roland S.**; Seibert, Karen
PA USA
SO U.S., 28 pp., Cont.-in-part of U.S. Ser. No. 387,680, abandoned.
CODEN: USXXAM
DT Patent
LA English
IC ICM C07D261-06
ICS C07D261-10; C07D261-12; C07D261-14; A61K031-42
NCL 514378000
CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO:	DATE
PI	US 5633272	A	19970527	US 1995-473884	19950607 <--
	CA 2212836	AA	19960822	CA 1996-2212836	19960212 <--
	CA 2212836	C	20030812		
	WO 9625405	A1	19960822	WO 1996-US1869	19960212 <--
	W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR				
	AU 9648671	A1	19960904	AU 1996-48671	19960212 <--
	AU 699593	B2	19981210		
	BR 9607035	A	19971104	BR 1996-7035	19960212 <--
	EP 809636	A1	19971203	EP 1996-904614	19960212 <--
	EP 809636	B1	20020904		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE				
	CN 1181075	A	19980506	CN 1996-193240	19960212 <--
	CN 1107058	B	20030430		
	JP 11503722	T2	19990330	JP 1996-525057	19960212 <--
	JP 3267300	B2	20020318		
	JP 2002179656	A2	20020626	JP 2001-326343	19960212 <--
	EP 1223167	A2	20020717	EP 2002-3253	19960212 <--
	EP 1223167	A3	20020807		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE				
	AT 223390	E	20020915	AT 1996-904614	19960212 <--
	PT 809636	T	20021231	PT 1996-904614	19960212 <--

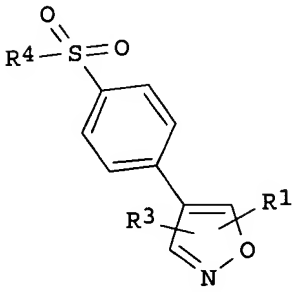
RU 2200158	C2	20030310	RU 1997-115452	19960212	<--
ES 2183935	T3	20030401	ES 1996-904614	19960212	<--
PL 185510	B1	20030530	PL 1996-321814	19960212	<--
PL 185544	B1	20030530	PL 1996-351239	19960212	<--
CZ 293211	B6	20040317	CZ 1997-2546	19960212	<--
ZA 9601150	A	19970212	ZA 1996-1150	19960213	<--
TW 449587	B	20010811	TW 1996-85109684	19960809	<--
US 5859257	A	19990112	US 1996-702417	19960814	<--
US 5985902	A	19991116	US 1997-801768	19970218	<--
FI 9703292	A	19970811	FI 1997-3292	19970811	<--
NO 9703711	A	19971006	NO 1997-3711	19970812	<--
CN 1442139	A	20030917	CN 2003-107042	20030228	<--
PRAI US 1995-387680	B2	19950213	<--		
US 1995-473884	A	19950607	<--		
EP 1996-904614	A3	19960212	<--		
JP 1996-525057	A3	19960212	<--		
WO 1996-US1869	W	19960212	<--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 5633272	ICM	C07D261-06
	ICS	C07D261-10; C07D261-12; C07D261-14; A61K031-42
	NCL	514378000

OS MARPAT 127:65756

GI



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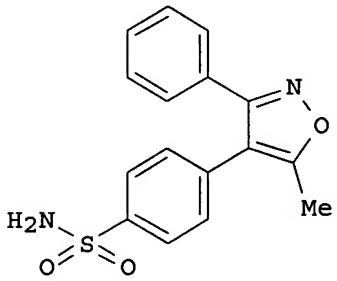


II

AB The title compds. [I; R1 = alkyl, carboxyalkyl, alkoxyalkyl, etc.; R3 = (un)substituted cycloalkyl, cycloalkenyl, aryl; R4 = lower alkyl, OH, NH2], useful in treatment of inflammation and inflammation-associated disorders such as arthritis, pain, and fever, were prepared Thus, treatment of desoxybenzoin oxime with BuLi/hexanes in THF followed by addition of Ac2O, reaction of the resulting 3,4-diphenyl-4-hydro-5-hydroxy-5-methylisoxazole with ClSO3H, and treatment of the intermediate with saturated NH4OH solution afforded 30% II which showed ID50 of < 0.1 μM against **COX-2.**

ST isoxazole prepn antiinflammatory; antiarthritic isoxazole prepn; analgesic isoxazole prepn; antipyretic isoxazole prepn; **cyclooxygenase** inhibitor isoxazole prepn

IT **Analgesics**
Anti-inflammatory agents
Antiarthritics
Antipyretics
(preparation of substituted isoxazoles for the treatment of inflammation)

IT **39391-18-9**
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(**COX-2** inhibitors; preparation of substituted isoxazoles for the treatment of inflammation)

IT **181695-72-7P 181695-81-8P**

RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of substituted isoxazoles for the treatment of inflammation)

IT **181695-73-8P 181695-74-9P 181695-75-0P**
181695-76-1P 181695-78-3P 181695-79-4P
181695-80-7P 181695-82-9P 181695-83-0P
181695-84-1P 181696-24-2P 181696-25-3P
181696-26-4P 181696-27-5P 181696-28-6P
181696-29-7P 181696-30-0P 181696-31-1P
181696-32-2P 181696-33-3P 181696-34-4P
181696-35-5P 181696-36-6P **181696-37-7P 181696-38-8P**
181696-39-9P 181696-40-2P 181696-41-3P
181696-42-4P 181696-43-5P 181696-44-6P
181696-45-7P 191421-97-3P 191421-98-4P
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted isoxazoles for the treatment of inflammation)

IT 71-43-2, Benzene, reactions 103-80-0, Phenylacetyl chloride 108-30-5, Succinic anhydride, reactions 321-28-8, 2-Fluoroanisole 451-40-1, Desoxybenzoin 766-51-8, 2-Chloroanisole 1722-69-6, 1,2-Diphenyl-1-buten-3-one 3446-89-7, 4-Methylthiobenzaldehyde 63327-11-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of substituted isoxazoles for the treatment of inflammation)

IT 325-62-2P 952-06-7P 3475-29-4P 13721-20-5P, 3-Chloro-4-methoxyphenylacetic acid 25632-70-6P 37612-52-5P 37928-17-9P 78967-09-6P 177560-74-6P 181696-73-1P 181696-74-2P 181696-75-3P 181696-76-4P **181696-77-5P** 181696-78-6P 181696-80-0P 181696-81-1P 181696-82-2P 181696-83-3P 181696-84-4P 181696-85-5P 181696-86-6P 181696-87-7P 181696-89-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of substituted isoxazoles for the treatment of inflammation)

IT **39391-18-9**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); MSC (Miscellaneous); **THU (Therapeutic use)**; **THU (Therapeutic use)**
(**COX-2** inhibitors; preparation of substituted isoxazoles for the treatment of inflammation)

RN 39391-18-9 HCAPLUS
CN Synthetase, prostaglandin endoperoxide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L102 ANSWER 17 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN **1997:361629** HCAPLUS
DN **126:330613**
ED Entered STN: 11 Jun 1997
TI Preparation of 1,3,5-trisubstituted pyrazoles for treatment of inflammation
IN Matsuo, Masaaki; Okumura, Kazuo; Ogino, Takashi; Nakamura, Katsuya; Nishimura, Hiroaki; Harada, Keiko; Hotta, Yuka; Tsuji, Kiyoshi
PA Fujisawa Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 54 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D231-12
ICS C07D231-14; A61K031-415; C07D231-16

CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

FAN.CNT 1

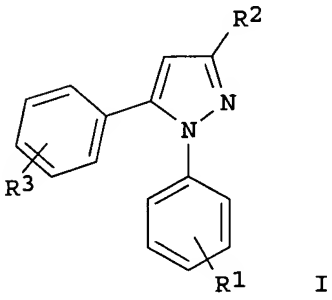
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9713755	A1	19970417	WO 1996-JP2919	19961008 <--
	W: AU, CA, CN, HU, IL, JP, KR, MX, US, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	ZA 9608286	A	19970513	ZA 1996-8286	19961002 <--
	CA 2234511	AA	19970417	CA 1996-2234511	19961008 <--
	AU 9671461	A1	19970430	AU 1996-71461	19961008 <--
	EP 856000	A1	19980805	EP 1996-932841	19961008 <--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
	CN 1203589	A	19981230	CN 1996-198649	19961008 <--
	JP 11513403	T2	19991116	JP 1996-514909	19961008 <--
PRAI	GB 1995-20584	A	19951009 <--		
	WO 1996-JP2919	W	19961008		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 9713755	ICM	C07D231-12
	ICS	C07D231-14; A61K031-415; C07D231-16

OS MARPAT 126:330613

GI



I

AB The title compds. [I; R1 = hydroxyethyl, 1-hydroxy-1-methylethyl, H, halo, NO2, CN; R2 = Cl, CN, lower alkyl optionally substituted with halogen; R3 = lower alkylthio, lower alkylsulfinyl, lower alkylsulfonyl], COX-II inhibitors and useful in the treatment and/or prevention of inflammatory conditions, various pains, collagen diseases, autoimmune diseases, various immunity diseases, thrombosis, cancer or neurodegenerative diseases, were prepared Thus, treatment of 3-chloro-1-(4-chlorophenyl)-5-[4-(methylthio)phenyl]pyrazole with m-chloroperbenzoic acid in CH2Cl2 afforded I [R1 = 4-Cl; R2 = Cl; R3 = 4-(MeSO2)] which showed at 3.2 mg/kg inhibition of secondary lesion of ≥ 95% in female Sprague-Dawley rats injected with Mycobacterium tuberculosis (strain M37 BA).

ST pyrazole prepn **cyclooxygenase** COXII inhibitor; antiinflammatory pyrazole prepn; analgesic pyrazole prepn; collagen disease pyrazole prepn; autoimmune disease pyrazole prepn; immunity disease pyrazole prepn; thrombosis pyrazole prepn; anticancer drug pyrazole prepn; neurodegenerative disease pyrazole prepn

IT Nervous system
(degeneration, treatment of; preparation of 1,3,5-trisubstituted pyrazoles for treatment of inflammation)

IT Connective tissue
(disease, treatment of; preparation of 1,3,5-trisubstituted pyrazoles for treatment of inflammation)

IT Immunity
(disorder, treatment of; preparation of 1,3,5-trisubstituted pyrazoles for treatment of inflammation)
IT **Analgesics**
Anti-inflammatory agents
Antitumor agents
(preparation of 1,3,5-trisubstituted pyrazoles for treatment of inflammation)
IT Autoimmune disease
Thrombosis
(treatment of; preparation of 1,3,5-trisubstituted pyrazoles for treatment of inflammation)
IT **39391-18-9, Cyclooxygenase**
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(COX-II inhibitors; preparation of 1,3,5-trisubstituted pyrazoles for treatment of inflammation)
IT 189699-66-9P 189699-77-2P 189699-79-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 1,3,5-trisubstituted pyrazoles for treatment of inflammation)
IT 151506-85-3P **189699-63-6P** 189699-64-7P **189699-65-8P**
189699-67-0P 189699-68-1P **189699-69-2P** 189699-70-5P
189699-71-6P 189699-72-7P 189699-73-8P 189699-74-9P
189699-75-0P 189699-76-1P 189699-78-3P 189699-80-7P
189699-81-8P 189699-82-9P 189699-83-0P
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189699-88-5P 189699-89-6P 189699-90-9P 189699-91-0P
189699-92-1P 189699-93-2P 189699-94-3P
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1,3,5-trisubstituted pyrazoles for treatment of inflammation)
IT 99-92-3 24654-52-2 35467-71-1, 4-Chlorophenylhydrazine hydrochloride
128172-84-9 134731-37-6 134754-00-0 151506-50-2 **151506-61-5**
151506-86-4 151507-00-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 1,3,5-trisubstituted pyrazoles for treatment of inflammation)
IT **151506-59-1P** 151506-84-2P 189699-95-4P 189699-96-5P
189699-97-6P **189699-98-7P 189699-99-8P** 189700-00-3P
189700-01-4P 189700-02-5P 189700-03-6P 189700-04-7P 189700-05-8P
189700-06-9P 189700-07-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1,3,5-trisubstituted pyrazoles for treatment of inflammation)
IT **39391-18-9, Cyclooxygenase**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); MSC (Miscellaneous); **THU (Therapeutic use)**; PROC (Process)
(COX-II inhibitors; preparation of 1,3,5-trisubstituted pyrazoles for treatment of inflammation)
RN 39391-18-9 HCAPLUS
CN Synthetase, prostaglandin endoperoxide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L102 ANSWER 18 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:342369 HCAPLUS
DN 126:317377
ED Entered STN: 31 May 1997
TI Preparation of substituted pyrazolylbenzenesulfonamides for use in veterinary therapies as antiinflammatory agents
IN Isakson, Peter C.; **Talley, John J.**
PA **G.D. Searle** and Co., USA; Isakson, Peter C.; Talley, John J.
SO PCT Int. Appl., 214 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM A61K031-635
ICS A61K031-415
CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	WO 9711704	A1	19970403	WO 1996-US15538	19960927	<--
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	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM					
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	CA 2233620	AA	19970403	CA 1996-2233620	19960927	<--
	AU 9673768	A1	19970417	AU 1996-73768	19960927	<--
	AU 718300	B2	20000413			
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	JP 11514991	T2	19991221	JP 1996-513685	19960927	<--
	AT 238058	E	20030515	AT 1996-936018	19960927	<--
	IL 123635	A1	20030624	IL 1996-123635	19960927	<--
	PT 854723	T	20030829	PT 1996-936018	19960927	<--
	ES 2197954	T3	20040116	ES 1996-936018	19960927	<--
	NO 9801392	A	19980525	NO 1998-1392	19980327	<--
	BR 9610974	A	19990713	BR 1996-10974	19980330	<--
PRAI	US 1995-536318	A1	19950929	<--		
	WO 1996-US15538	W	19960927			

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES	
WO 9711704	ICM	A61K031-635	
	ICS	A61K031-415	
WO 9711704	ECLA	A61K031/415; A61K031/635	<--
US 5756529	ECLA	A61K031/415; A61K031/635	<--

OS MARPAT 126:317377
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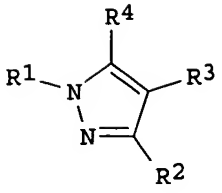

I

AB The title compds. [I; R1 = substituted aryl (e.g., 4-(H2NSO2)C6H4), heteroaryl; R2 = H, halo, alkyl, etc.; R3 = H, alkyl, halo, etc.; R4 = (un)substituted aralkenyl, aryl, cycloalkyl, etc.], useful in treating inflammation and inflammation-related disorders (e.g., arthritis and pain) in animals, were prepared Thus, reaction of Et trifluoroacetate with 4'-chloroacetophenone in the presence NaOMe in Me tert-Bu ether followed by cyclization of the resulting of 4,4,4-trifluoro-1-(4-chlorophenyl)butane-1,3-dione with 4-sulfonamidophenylhydrazine.HCl in EtOH afforded I [R1 = 4-(H2NSO2)C6H4; R2 = CF3; R3 = H; R4 = 4-ClC6H4] which showed ID50 of <0.1 μM against human **cyclooxygenase** II.

ST pyrazolylbenzenesulfonamide prepn antiinflammatory veterinary; antiarthritic veterinary pyrazolylbenzenesulfonamide prepn; analgesic veterinary pyrazolylbenzenesulfonamide prepn; **cyclooxygenase** inhibitor pyrazolylbenzenesulfonamide prepn

IT **Analgesics**
Anti-inflammatory agents
Antiarthritics
(preparation of substituted pyrazolylbenzenesulfonamides for use in veterinary therapies as antiinflammatory agents)

IT Drugs
(veterinary; preparation of substituted pyrazolylbenzenesulfonamides for use in veterinary therapies as antiinflammatory agents)

IT **39391-18-9, Cyclooxygenase**
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(COX II inhibitors; preparation of substituted pyrazolylbenzenesulfonamides for use in veterinary therapies as antiinflammatory agents)

IT **169590-42-5P 170569-52-5P 170569-86-5P**
170570-11-3P 170570-25-9P 170570-26-0P
170570-27-1P 170570-47-5P 170570-52-2P
170570-56-6P 170570-80-6P 170571-00-3P
170571-19-4P 170571-20-7P 170571-29-6P
170571-74-1P
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of substituted pyrazolylbenzenesulfonamides for use in veterinary therapies as antiinflammatory agents)

IT **970-12-7P 169590-41-4P 170569-22-9P**
170569-23-0P 170569-25-2P 170569-26-3P
170569-27-4P 170569-28-5P 170569-29-6P
170569-30-9P 170569-31-0P 170569-32-1P
170569-33-2P 170569-34-3P 170569-35-4P
170569-36-5P 170569-37-6P 170569-38-7P
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170569-45-6P 170569-46-7P 170569-47-8P
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170572-09-5P **170572-10-8P**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted pyrazolylbenzenesulfonamides for use in veterinary therapies as antiinflammatory agents)

IT 170572-11-9P **170572-13-1P 170572-15-3P**
188816-93-5P 189346-78-9P 189346-80-3P
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted pyrazolylbenzenesulfonamides for use in veterinary therapies as antiinflammatory agents)

IT 93-55-0, Propiophenone 96-48-0, γ-Butyrolactone 98-86-2, Acetophenone, reactions 99-91-2, 4'-Chloroacetophenone 100-06-1 100-58-3 105-56-6, Ethyl cyanoacetate 106-31-0, Butyric anhydride 108-42-9, 3-Chloroaniline 122-00-9, 4'-Methylacetophenone 137-06-4, o-Thiocresol 321-28-8, 2-Fluoroanisole 356-27-4, Ethyl heptafluorobutyrate 403-42-9, 4'-Fluoroacetophenone 437-82-1, 2,6-Difluoroanisole 488-17-5, 3-Methylcatechol 529-34-0, 1-Tetralone 553-90-2, Dimethyl oxalate 578-58-5, 2-Methylanisole 582-24-1, 2-Hydroxyacetophenone 823-85-8, 4-Fluorophenylhydrazine hydrochloride 1132-05-4, 3-Allyl-4-hydroxyacetophenone 1565-17-9, 4-(Aminosulfonyl)acetophenone 1984-65-2, 2,6-Dichloroanisole 2687-43-6, O-Benzylhydroxylamine hydrochloride 2746-25-0, 4-Methoxybenzyl bromide 2892-18-4, 5-Methyl-1-phenyl-1-hexen-3-one 3162-29-6 4653-11-6, 4-(2-Thienyl)butyric acid 7051-34-5, (Bromomethyl)cyclopropane 14804-32-1, 2-Ethylanisole 17852-52-7 22047-25-2, Acetylpyrazine 51015-29-3, 6-Methyl-1-tetralone
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of substituted pyrazolylbenzenesulfonamides for use in veterinary therapies as antiinflammatory agents)

IT 318-46-7P, 2-Trifluoroacetyl-1-tetralone 322-06-5P 450-95-3P, 2-Fluoroacetophenone 455-91-4P 720-94-5P 2388-73-0P, 2-Methylthioanisole 13414-95-4P 18931-60-7P 20487-10-9P 20577-73-5P 23894-54-4P 29643-34-3P 29665-52-9P 39757-34-1P 39757-35-2P 41727-59-7P 56856-73-6P 63301-25-7P 100256-35-7P 106876-38-4P 142499-46-5P 164342-68-1P **170570-75-9P** 170570-76-0P 170570-77-1P 170570-78-2P 170570-79-3P **170570-81-7P** 170570-82-8P **170570-83-9P** 170570-85-1P 170570-86-2P **170570-88-4P** 170570-90-8P **170570-91-9P** **170570-94-2P** 170570-95-3P 170570-96-4P 188817-19-8P 189347-36-2P 189347-40-8P 189347-42-0P 189347-51-1P **189347-54-4P** 189347-56-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of substituted pyrazolylbenzenesulfonamides for use in veterinary therapies as antiinflammatory agents)

IT 170570-87-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of substituted pyrazolylbenzenesulfonamides for use in veterinary therapies as antiinflammatory agents)

IT **39391-18-9, Cyclooxygenase**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); MSC (Miscellaneous); **THU (Therapeutic use)**; **THU (Therapeutic use)**
(COX II inhibitors; preparation of substituted pyrazolylbenzenesulfonamides for use in veterinary therapies as antiinflammatory agents)

RN 39391-18-9 HCAPLUS
CN Synthetase, prostaglandin endoperoxide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L102 ANSWER 19 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:94058 HCAPLUS
DN 126:104081
ED Entered STN: 10 Feb 1997
TI Substituted sulfonylphenylheterocycles as **cyclooxygenase-2** and **5-lipoxygenase** inhibitors
IN **Rogers, Roland S.**; **Talley, John J.**; **Sikorski, James A.**; **Devadas, Balekudru**; **Graneto, Matthew J.**; **Carter, Jeffery S.**; **Norman, Bryan H.**; **Lu, Hwang-fun**; **Brown, David L.**; Nagarajan, Srinivasan
PA **G.D. Searle** and Co., USA; Rogers, Kathy, L.; Talley, John J.; Sikorski, James A.; Devadas, Balekudru; Graneto, Matthew J.; Carter, Jeffery S.; Norman, Bryan H.; Lu, Hwang-Fun; et al.
SO PCT Int. Appl., 181 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D405-12
ICS C07D413-12; C07D231-12; A61K031-42; A61K031-415
CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9638442	A1	19961205	WO 1996-US8183	19960531 <--
	W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI				
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	AU 9660279	A1	19961218	AU 1996-60279	19960531 <--
	EP 828736	A1	19980318	EP 1996-917888	19960531 <--
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	PT 995747	T	20021231	PT 2000-100201	19960531 <--
	ES 2181614	T3	20030301	ES 2000-100201	19960531 <--
	AT 246188	E	20030815	AT 1996-917888	19960531 <--
	PT 828736	T	20031231	PT 1996-917888	19960531 <--
	ES 2205035	T3	20040501	ES 1996-917888	19960531 <--
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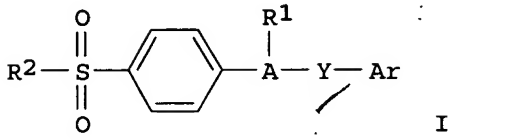
PRAI	US 1995-460324	A	19950602 <--		
	EP 1996-917888	A3	19960531 <--		
	WO 1996-US8183	W	19960531 <--		
	US 1998-952661	B1	19980420 <--		
	US 2000-549830	B1	20000414 <--		
	US 2001-4960	A1	20011204		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 9638442	ICM	C07D405-12
	ICS	C07D413-12; C07D231-12; A61K031-42; A61K031-415

OS MARPAT 126:104081
GI



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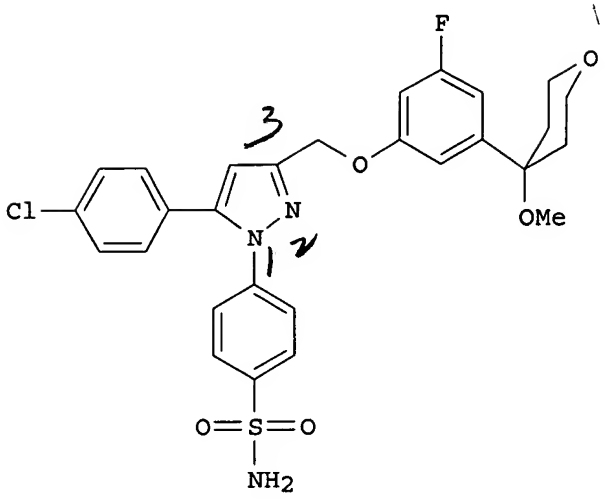

II

AB The invention relates to antiinflammatory pharmaceutical agents, specifically to compds. I and their pharmaceutically acceptable salts, their compns., and methods for treating disorders mediated by **cyclooxygenase-2** (**COX-2**) or **5-lipoxygenase** (5-LO), such as inflammation [wherein A = 5- or 6-membered, (un)saturated, (un)substituted hetero- or carbocycle; Y = O, S, S(O), S(O)2, alk(en/yn)yl, alkoxy, alk(en/yn)ylthio, many others; Ar = (un)substituted (hetero)aryl; R1 = 1 or more (un)substituted heterocyclyl, cycloalk(en)yl, or aryl; R2 = alkyl, amino]. For instance, condensation of di-Me oxalate with 4-ClC6H4COMe gave 54.4% 4-ClC6H4COCH2COCO2Me. This underwent a sequence of: (1) cyclocondensation with 4-H2NSO2C6H4NHNH2.HCl to give a pyrazolecarboxylate ester (90%); (2) alkaline saponification of ester (94%); (3) reduction of the acid with BH3.THF to a hydroxymethyl compound (71%); (4) conversion of the latter to a mesylate, and etherification of the mesylate with a phenol derivative (25%), to give title compound II. In vitro assays of II showed IC50 values (μM) of <0.1 for **COX-2**, 38 for **COX-1**, and 0.15 for 5-LO.

ST sulfonylphenylheterocycle prepn inhibitor **cyclooxygenase** lipoxygenase; antiinflammatory pyrazole oxazole sulfonylphenyl prepn

IT **Allergy inhibitors**
Analgesics
Anti-inflammatory agents
Antiarthritics
Antiasthmatics
Antipyretics
(preparation of substituted sulfonylphenylheterocycles as **cyclooxygenase-2** and **5-lipoxygenase** inhibitors)

IT 5014-83-5P 39757-35-2P, Methyl 4-(4-chlorophenyl)-2,4-dioxobutanoate 49656-04-4P 130723-29-4P **163303-46-6P 163303-48-8P**

163304-74-3P 163304-95-8P **170571-19-4P**
170571-20-7P **170571-71-8P** **181696-34-4P**
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185343-22-0P **185343-27-5P** 185345-56-6P 185345-57-7P
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185965-86-0P 185965-87-1P 185965-88-2P 185965-89-3P 185965-90-6P
185965-91-7P **185965-92-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of substituted sulfonylphenylheterocycles as **cyclooxygenase-2** and **5-lipoxygenase** inhibitors)

IT **185965-32-6P** **185965-33-7P** **185965-34-8P**
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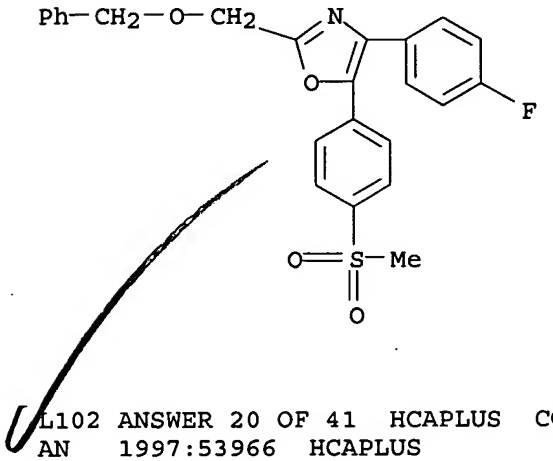
185965-47-3P **185965-48-4P** **185965-49-5P**
185965-50-8P **185965-51-9P** **185965-52-0P**
185965-53-1P **185965-54-2P** **185965-55-3P**
185965-56-4P **185965-57-5P** **185965-58-6P**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted sulfonylphenylheterocycles as **cyclooxygenase-2** and **5-lipoxygenase** inhibitors)

IT **39391-18-9**, **Cyclooxygenase** **80619-02-9**, **5-Lipoxygenase**
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(preparation of substituted sulfonylphenylheterocycles as **cyclooxygenase-2** and **5-lipoxygenase** inhibitors)

IT 51-79-6, Urethane 96-35-5, Methyl glycolate 99-91-2, 4'-Chloroacetophenone 105-36-2, Ethyl bromoacetate 106-96-7, Propargyl bromide 119-53-9, Benzoin 124-63-0, Methanesulfonyl chloride 347-84-2 451-40-1, Deoxybenzoin 553-90-2, Dimethyl oxalate 1798-06-7, 4-Iodophenylacetic acid 2304-94-1 2365-48-2, Methyl thioglycolate 2417-72-3, Methyl 4-(bromomethyl)benzoate 2836-32-0, Glycolic acid monosodium salt 2935-90-2, Methyl 3-mercaptopropionate 15570-12-4, 3-Methoxythiophenol 17852-52-7, Benzenesulfonamide, 4-hydrazino-, monohydrochloride 19810-31-2, Benzyloxyacetyl chloride 52267-39-7, Benzyl methyl malonate 121148-97-8 130722-57-5 130723-09-0 144800-91-9 161446-59-9 163303-22-8 **181695-72-7** 185965-93-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of substituted sulfonylphenylheterocycles as **cyclooxygenase-2** and **5-lipoxygenase** inhibitors)

IT **163303-46-6P**
RL: **BAC (Biological activity or effector, except adverse)**; SPN (Synthetic preparation); PREP (Preparation); **THU (Therapeutic use)**
(intermediate; preparation of substituted sulfonylphenylheterocycles as **cyclooxygenase-2** and **5-lipoxygenase** inhibitors)

RN 163303-46-6 HCAPLUS
CN Oxazole, 4-(4-fluorophenyl)-5-[4-(methylsulfonyl)phenyl]-2-[(phenylmethoxy)methyl]- (9CI) (CA INDEX NAME)



L102 ANSWER 20 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:53966 HCAPLUS
DN 126:74828
ED Entered STN: 25 Jan 1997
TI Preparation of substituted oxazoles as antiinflammatories.
IN **Talley, John J.**; Bertenshaw, Stephen; Rogier, Donald J., Jr.; **Graneto, Matthew**; **Brown, David L.**; **Devadas, Balekudru**; **Lu, Hwang-Fun**; **Sikorski, James A.**
PA **G.D. Searle** and Co., USA
SO PCT Int. Appl., 243 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D263-32
ICS A61K031-42; C07D413-06; C07D413-10; C07D263-34; C07D263-38; C07D263-46; C07D263-48; C07F009-653
CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))
FAN.CNT 3

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9636617	A1	19961121	WO 1996-US6992	19960516 <--
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN				
CA 2221692	AA	19961121	CA 1996-2221692	19960516 <--
AU 9658603	A1	19961129	AU 1996-58603	19960516 <--
EP 825989	A1	19980304	EP 1996-920231	19960516 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
JP 11509835	T2	19990831	JP 1996-535029	19960516 <--
PRAI US 1995-445312	A	19950519 <--		
WO 1996-US6992	W	19960516 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 9636617	ICM	C07D263-32
	ICS	A61K031-42; C07D413-06; C07D413-10; C07D263-34; C07D263-38; C07D263-46; C07D263-48; C07F009-653

OS MARPAT 126:74828
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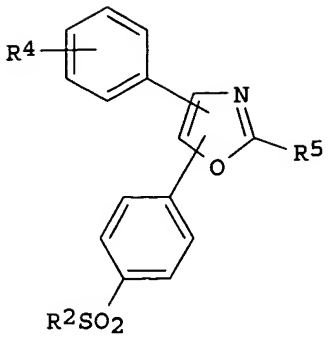

I

AB Title compds. (I; R2 = alkyl, amino; R4 = H, alkyl, alkylamino, alkoxy, halo; R5 = halo, SH, carboxyalkylthio, aminocarbonyl, amino acid residue, haloalkoxy, aryloxy, phosphonylalkyl, cyanoalkyl, heterocyclylalkyl, etc.), were prepared Thus, 4-(4-fluorophenyl)-2-(2-phenylethyl)-5-(4-methylsulfonyphenyl)oxazole, prepared from 1-(4-fluorophenyl)-2-(4-methylthiophenyl)ethanone, at 10 mg/kg gave 41% inhibition of edema in the carrageenan foot pad edema test.

ST oxazole phenyl prepn antiinflammatory; sulfonylphenyloxazole prepn antiinflammatory; analgesic sulfonylphenyloxazole

IT **Analgesics**
Anti-inflammatory agents
Antiarthritics
Antipyretics
(preparation of substituted oxazoles as antiinflammatories)

IT **39391-18-9**
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(2, inhibitors; preparation of substituted oxazoles as antiinflammatories)

IT **92872-92-9P 92873-57-9P 93014-16-5P**
93014-17-6P 163303-18-2P 163303-19-3P
163303-25-1P 163303-26-2P 163303-27-3P
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RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted oxazoles as antiinflammatories)

IT 51-79-6, Urethane 72-17-3, Lactic acid sodium salt 74-88-4, Methyl iodide, reactions 75-89-8, 2,2,2-Trifluoroethanol 98-88-4, Benzoyl chloride 100-39-0, Benzyl bromide 100-58-3 104-87-0, 4-Methylbenzaldehyde 104-88-1, 4-Chlorobenzaldehyde, reactions 104-95-0, 4-Bromothioanisole 108-43-0, 3-Chlorophenol 108-95-2, Phenol, reactions 118-61-6, Ethyl salicylate 119-53-9, Benzoin 124-40-3, Dimethylamine, reactions 124-41-4, Sodium methoxide 124-63-0, Methanesulfonyl chloride 347-84-2 351-54-2, 3-Fluoro-p-anisaldehyde 353-85-5, Trifluoroacetonitrile 367-51-1, Mercaptoacetic acid sodium salt 371-41-5, 4-Fluorophenol 381-73-7, Difluoroacetic acid 405-50-5, 4-Fluorophenylacetic acid 451-40-1, Deoxybenzoin 456-48-4, 3-Fluorobenzaldehyde 459-57-4, 4-Fluorobenzaldehyde 627-91-8, Adipic acid monomethyl ester 645-45-4, Hydrocinnamoyl chloride 696-59-3, 2,5-Dimethoxytetrahydrofuran 771-61-9, Pentafluorophenol 922-67-8, Methyl propiolate 1663-39-4, tert-Butyl acrylate 1798-06-7, 4-Iodophenylacetic acid 2033-24-1,

2,2-Dimethyl-1,3-dioxane-4,6-dione 2043-61-0, Cyclohexanecarboxaldehyde 2365-48-2, Methyl thioglycolate 2836-32-0, Glycolic acid monosodium salt 3446-89-7, 4-Methylthiobenzaldehyde 4294-57-9, 4-Methylphenylmagnesium bromide 5188-07-8, Sodium thiomethoxide 5672-83-3 5781-53-3, Methyl oxalyl chloride 6287-38-3, 3,4-Dichlorobenzaldehyde 6317-85-7, 4-Dimethylaminobenzoin 7677-24-9, Trimethylsilyl cyanide 7781-98-8, Ethyl 3-hydroxybenzoate 14224-99-8, 2-Methyl-4,5-diphenyloxazole 19810-31-2, Benzyloxyacetyl chloride 21256-18-8, 4,5-Diphenyl-2-oxazolepropionic acid 25438-37-3 27151-66-2 34036-07-2, 3,4-Difluorobenzaldehyde 34328-61-5, 3-Chloro-4-fluorobenzaldehyde 35444-44-1, 5-Methoxycarbonylpentanoyl chloride 36239-09-5, Ethyl malonyl chloride 38870-89-2, Methoxyacetyl chloride 39098-75-4, Cyclohexanepropanoyl chloride 87483-29-2 **163303-34-2** **163304-87-8** 163304-91-4 185345-87-3 185345-88-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of substituted oxazoles as antiinflammatories)

IT 2431-02-9P 2431-23-4P 4675-18-7P 5014-83-5P 36187-57-2P
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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of substituted oxazoles as antiinflammatories)

IT **39391-18-9**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); MSC (Miscellaneous); **THU (Therapeutic use)**; PROC (Process)
(2, inhibitors; preparation of substituted oxazoles as antiinflammatories)

RN 39391-18-9 HCAPLUS
CN Synthetase, prostaglandin endoperoxide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L102 ANSWER 21 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:601794 HCAPLUS
DN 125:247800
ED Entered STN: 10 Oct 1996
TI Substituted isoxazoles for the treatment of inflammation
IN **Rogers, Roland S.**; **Talley, John J.**; **Brown, David L.**; Nagarajan, Srinivasan; **Carter, Jeffery S.**; Weier, Richard M.; Stealey, Michael A.; Collins, Paul W.; Seibert, Karen; et al.
PA **G.D. Searle** and Co., USA; Rogers, Kathy L.

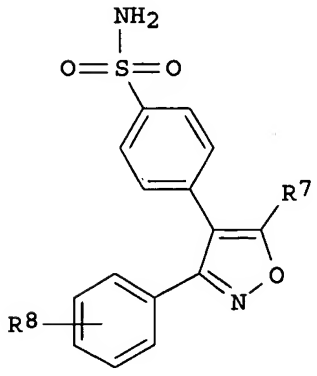
SO PCT Int. Appl., 171 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D261-08
ICS C07D413-04; C07D261-18; C07D261-12; C07D261-10; A61K031-42
CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 3

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9625405	A1	19960822	WO 1996-US1869	19960212 <--
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR				
US 5633272	A	19970527	US 1995-473884	19950607 <--
AU 9648671	A1	19960904	AU 1996-48671	19960212 <--
AU 699593	B2	19981210		
BR 9607035	A	19971104	BR 1996-7035	19960212 <--
EP 809636	A1	19971203	EP 1996-904614	19960212 <--
EP 809636	B1	20020904		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE				
JP 11503722	T2	19990330	JP 1996-525057	19960212 <--
JP 3267300	B2	20020318		
AT 223390	E	20020915	AT 1996-904614	19960212 <--
RU 2200158	C2	20030310	RU 1997-115452	19960212 <--
PL 185510	B1	20030530	PL 1996-321814	19960212 <--
PL 185544	B1	20030530	PL 1996-351239	19960212 <--
FI 9703292	A	19970811	FI 1997-3292	19970811 <--
NO 9703711	A	19971006	NO 1997-3711	19970812 <--
PRAI US 1995-387680	A2	19950213 <--		
US 1995-473884	A2	19950607 <--		
WO 1996-US1869	W	19960212 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 9625405	ICM	C07D261-08
	ICS	C07D413-04; C07D261-18; C07D261-12; C07D261-10; A61K031-42

OS MARPAT 125:247800
GI



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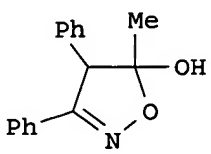

II

AB A class of substituted isoxazolyl compds. is described, for use in treatment of inflammation and inflammation-related disorders. Compds. of particular interest are I [R7 = OH, (un)substituted alkyl, CO2H, halo, cycloalkyl, cycloalkylalkyl, and aralkyl; R8 = 1 or more H, alkylsulfinyl, alkyl, cyano, CO2H, alkoxycarbonyl, haloalkyl, OH, hydroxyalkyl, haloalkoxy, amino, alkylamino, arylamino, aminoalkyl, NO2, halo, alkoxy, aminosulfonyl, and alkylthio] and their pharmaceutically-acceptable salts. For example, PhCOCH2Ph was converted to the oxime (82%), and this was lithiated with BuLi, acetylated with Ac2O, and cyclized to give the oxazoline derivative II. This compound underwent dehydration and chlorosulfonylation with ClSO3H, followed by ammonolysis with aqueous NH3, to give I [R7 = Me, R8 =H]. Lithiation of the latter with BuLi, oxygenation with O2, and reductive workup with P(OMe)3, gave title compound I [R7 = CH2OH, R8 = H] (III). At 10 mg/kg orally in rats, III gave 57% and 74% inhibition in the carrageenan-induced paw edema and analgesia tests, resp. I selectively inhibited **cyclooxygenase 2 (COX -2)** over **COX-1** in vitro, with typical IC50 values of 0.1-5.0 μM and >100 μM, resp.

ST isoxazole prepn antiinflammatory analgesic antiarthritic antipyretic; benzenesulfonamide isoxazolyl prepn **cyclooxygenase 2** inhibitor

IT **Analgesics**
Antipyretics
Inflammation inhibitors
(preparation of substituted isoxazoles as antiinflammatories)

IT **Inflammation inhibitors**
(**antiarthritics**, preparation of substituted isoxazoles as antiinflammatories)

IT **39391-18-9**
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(2, inhibitors; preparation of substituted isoxazoles as antiinflammatories)

IT 325-62-2P 952-06-7P 1023-17-2P 2001-28-7P 2001-29-8P 3475-29-4P 6318-76-9P 13721-20-5P, 3-Chloro-4-methoxyphenylacetic acid 16736-09-7P 16736-13-3P 16737-10-3P 25632-70-6P 25870-62-6P, 1-Phenyl-2-hexanone 37612-52-5P 37928-17-9P, 3,4-Diphenyl-5-methylisoxazole 62482-45-5P 78967-09-6P 104896-80-2P 121411-85-6P 177560-73-5P 177560-74-6P 177561-49-8P 181696-73-1P 181696-74-2P 181696-75-3P 181696-76-4P 181696-78-6P 181696-79-7P 181696-80-0P 181696-81-1P 181696-82-2P 181696-83-3P 181696-84-4P 181696-85-5P 181696-86-6P 181696-87-7P 181696-88-8P 181696-89-9P 181696-90-2P 181696-91-3P, 4,5-Diphenyl-3-ethylisoxazole 181696-92-4P 181696-93-5P 181696-94-6P 181696-95-7P 181696-96-8P 181696-97-9P 181696-98-0P 181696-99-1P 181697-00-7P 181697-01-8P 181697-02-9P 181697-03-0P 181697-04-1P 181697-05-2P 181697-06-3P 181697-07-4P 181697-08-5P 181697-09-6P 181697-10-9P 181697-11-0P 181697-12-1P 181697-13-2P **181697-14-3P** 181697-15-4P 181697-16-5P 181697-17-6P 181697-18-7P 181697-19-8P 181697-20-1P 181697-21-2P 181697-22-3P 181697-23-4P 181697-24-5P 181697-25-6P 181697-26-7P 181697-27-8P 181697-28-9P 181697-29-0P 181697-30-3P 181697-31-4P 181697-32-5P 181697-33-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of substituted isoxazoles as antiinflammatories)

IT **181695-72-7P 181695-81-8P 181695-83-0P 181695-84-1P 181695-93-2P 181696-21-9P 181696-34-4P 181696-77-5P**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of substituted isoxazoles as antiinflammatories)

IT **181695-73-8P 181695-74-9P 181695-75-0P**
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RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted isoxazoles as antiinflammatories)

IT 71-43-2, Benzene, reactions 75-36-5, Acetyl chloride 99-76-3, Methyl 4-hydroxybenzoate 100-39-0, Benzyl bromide 100-52-7, Benzaldehyde, reactions 101-41-7, Methyl phenylacetate 103-79-7, Phenylacetone 103-80-0, Phenylacetyl chloride 104-87-0, p-Tolualdehyde 104-88-1, p-Chlorobenzaldehyde, reactions 108-24-7, Acetic anhydride 108-30-5, Succinic anhydride, reactions 108-55-4, Glutaric anhydride 108-89-4, 4-Picoline 110-13-4, Acetonylacetone 123-11-5, 4-Anisaldehyde, reactions 141-78-6, Ethyl acetate, reactions 321-28-8, 2-Fluoroanisole 358-23-6, Trifluoromethanesulfonic anhydride 383-63-1, Ethyl trifluoroacetate 446-52-6, 2-Fluorobenzaldehyde 451-40-1, Desoxybenzoin 454-31-9, Ethyl difluoroacetate 456-48-4, 3-Fluorobenzaldehyde 459-57-4, 4-Fluorobenzaldehyde 553-90-2, Dimethyl oxalate 587-04-2, 3-Chlorobenzaldehyde 620-23-5, 3-Methylbenzaldehyde 766-51-8, 2-Chloroanisole 925-90-6, Ethylmagnesium bromide 1007-32-5, 1-Phenyl-2-butanone 1122-91-4, 4-Bromobenzaldehyde 1722-69-6, 1,2-Diphenyl-1-buten-3-one 2893-05-2 3446-89-7, 4-(Methylthio)benzaldehyde 3795-79-7, Methyl 4-(methylthio)benzoate 4166-53-4, 3-Methylglutaric anhydride 4206-67-1, (Trimethylsilyl)iodomethane 4480-83-5, Diglycolic acid anhydride 5470-11-1, Hydroxylamine hydrochloride 6638-79-5, N,O-Dimethylhydroxylamine hydrochloride 6683-92-7, 1-Phenyl-2-pentanone 7677-24-9, Cyanotrimethylsilane 16188-55-9, 4-(Methylthio)phenylacetic acid 24424-99-5, Di-tert-butyl dicarbonate 32085-88-4, 3,5-Difluorobenzaldehyde 34036-07-2, 3,4-Difluorobenzaldehyde 63327-11-7 88356-92-7
RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; preparation of substituted isoxazoles as antiinflammatories)
IT **39391-18-9**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); MSC (Miscellaneous); **THU (Therapeutic use)**; **THU (Therapeutic use)**
(2, inhibitors; preparation of substituted isoxazoles as antiinflammatories)
RN 39391-18-9 HCAPLUS
CN Synthetase, prostaglandin endoperoxide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L102 ANSWER 22 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN **1996:520938** HCAPLUS
DN **125:167967**
ED Entered STN: 30 Aug 1996
TI Preparation of oxazole derivatives as selective **cyclooxygenase 2** inhibitors
IN Haruta, Junichi; Hashimoto, Hiromasa; Matsushita, Mutsuyoshi
PA Japan Tobacco Inc., Japan
SO PCT Int. Appl., 39 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
IC ICM C07D263-32
ICS C07D413-04; A61K031-42
CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9619462	A1	19960627	WO 1995-JP2588	19951215 <--
	W: CA, KR, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
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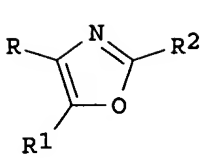
	CN 1146204	A	19970326	CN 1995-192620	19951218 <--
	US 5945539	A	19990831	US 1997-849879	19970618 <--
	US 6002014	A	19991214	US 1999-302498	19990430 <--
	US 2002143040	A1	20021003	US 2001-906761	20010718 <--
PRAI	JP 1994-335838	A	19941220	<--	
	JP 1995-93099	A	19950327	<--	
	JP 1995-108014	A	19950405	<--	
	JP 1995-164656	A	19950606	<--	
	JP 1995-326571	A	19951120	<--	
	WO 1995-JP2588	W	19951215	<--	
	CA 1995-2183645	A3	19951218	<--	
	US 2000-721705	A1	20001127		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 9619462	ICM	C07D263-32
	ICS	C07D413-04; A61K031-42

OS MARPAT 125:167967
GI



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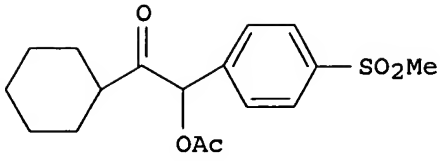
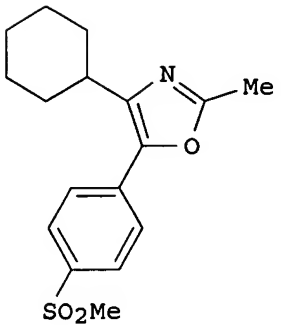


II



III

AB Oxazole derivs. represented by general formula (I; one of R and R1 represents methylsulfonylphenyl, aminosulfonylphenyl or alkylaminosulfonylphenyl, and the other of them represents C5-7 cycloalkyl which may be substituted by lower alkyl, thienyl which may be substituted by lower alkyl or halo, or furanyl which may be substituted by lower alkyl or halo; R2 represents lower alkyl) or medicinally acceptable salts thereof are prepared, each being excellent in antipyretic, analgesic, antiphlogistic, and particularly selective **cyclooxygenase-2** (**COX-2**) inhibitory effects and promising as an antipyretic, analgesic or antiinflammatory agent reduced in side effects such as gastrointestinal disturbance. Thus, coupling of cyclohexanecarbonyl chloride with 4-methylsulfonylbenzyl chloride in the presence of (Ph3P)4Pd and Zn powder in 1,2-dimethoxyethane at room temperature for 2 h and α-acetoxylation of the resulting cyclohexyl 4-methylsulfonylbenzyl ketone by Pb(OAc)4 in refluxing AcOH for 3 h gave a cyclohexylphenyloxazole intermediate (II), which was cyclocondensed with ammonium acetate in refluxing AcOH for 3 h to give the title compound (III). III in vitro showed IC50 of 0.07 and >100 μM against **cyclooxygenase 2** and 1, resp., as compared to 1.5 and 0.6 μM, resp., for indometacin and in vivo showed ED50 of 5.4 mg/kg p.o. for inhibiting carrageenan-induced edema in rats as compared to 2.9 mg/kg p.o. for indometacin.

ST oxazole prepn selective **cyclooxygenase 2** inhibitor; antipyretic analgesic antiinflammatory cyclohexylphenyloxazole

IT **Analgesics**
Antipyretics
Inflammation inhibitors
(preparation of oxazole derivs. as selective **cyclooxygenase 2** inhibitors, antipyretic, analgesic, or antiinflammatory agents)

IT **163303-47-7P 180302-37-8P 180302-38-9P**
180302-39-0P 180302-40-3P 180302-41-4P
180302-42-5P 180302-43-6P 180302-44-7P
180302-45-8P 180302-46-9P 180302-47-0P
180302-48-1P 180302-49-2P 180302-50-5P
180302-51-6P 180302-52-7P 180302-53-8P
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of oxazole derivs. as selective **cyclooxygenase 2** inhibitors, antipyretic, analgesic, or antiinflammatory

agents)

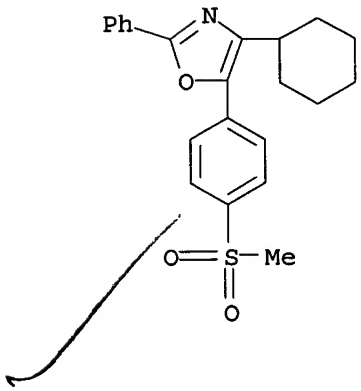
IT **39391-18-9**
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(preparation of oxazole derivs. as selective **cyclooxygenase 2** inhibitors, antipyretic, analgesic, or antiinflammatory agents)

IT 79-03-8, Propionyl chloride 100-44-7, Benzyl chloride, reactions 108-24-7, Acetic anhydride 631-61-8, Ammonium acetate 2719-27-9, Cyclohexanecarbonyl chloride 5470-11-1, Hydroxylamine hydrochloride 6213-85-0, Methyl p-bromobenzenesulfonate 6998-30-7, Methylamine acetate 7664-41-7, Ammonia, reactions 42518-98-9, 5-Chloro-2-thenoyl chloride 53606-06-7, 4-Methylsulfonylbenzyl bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of oxazole derivs. as selective **cyclooxygenase 2** inhibitors, antipyretic, analgesic, or antiinflammatory agents)

IT 546-67-8P, Lead tetraacetate 61259-29-8P, Benzyl cyclohexyl ketone 180302-54-9P 180302-55-0P 180302-56-1P 180302-57-2P 180302-58-3P 180302-59-4P 180302-60-7P 180302-61-8P 180302-62-9P 180302-63-0P, Cyclohexyl 4-methylsulfonylbenzyl ketone 180302-64-1P, Benzyl cyclohexyl ketone oxime
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of oxazole derivs. as selective **cyclooxygenase 2** inhibitors, antipyretic, analgesic, or antiinflammatory agents)

IT **163303-47-7P**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of oxazole derivs. as selective **cyclooxygenase 2** inhibitors, antipyretic, analgesic, or antiinflammatory agents)

RN 163303-47-7 HCAPLUS
CN Oxazole, 4-cyclohexyl-5-[4-(methylsulfonyl)phenyl]-2-phenyl- (9CI) (CA INDEX NAME)



L102 ANSWER 23 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN **1996:466918** HCAPLUS
DN **125:114611**
ED Entered STN: 08 Aug 1996
TI Pyrazole derivatives exhibiting anti-inflammatory and analgesic effects
IN Numata, Hirotoshi; Okamoto, Yasushi; Shinoda, Masanobu; Kobayashi, Naoki; Miyazawa, Shuhei; Kawahara, Tetsuya; Shirota, Hiroshi; Nagakura, Naoki; Horizoe, Tatsuo; et al.

PA Eisai Co., Ltd., Japan
SO PCT Int. Appl., 136 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D231-12
ICS A61K031-415; C07D401-06; C07D403-06; C07D403-10; C07D403-12; C07D405-04; C07D405-06; C07D405-10; C07D409-04; C07D409-06; C07D413-10; C07D417-06; C07D417-10
CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9614302	A1	19960517	WO 1995-JP2250	19951106 <--
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RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
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JP 10509140	T2	19980908	JP 1995-515193	19951106 <--
ZA 9509475	A	19960515	ZA 1995-9475	19951108 <--
PRAI JP 1994-274067	A	19941108 <--		
JP 1994-280705	A	19941115 <--		
JP 1995-48760	A	19950308 <--		
WO 1995-JP2250	W	19951106 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 9614302	ICM	C07D231-12
	ICS	A61K031-415; C07D401-06; C07D403-06; C07D403-10; C07D403-12; C07D405-04; C07D405-06; C07D405-10; C07D409-04; C07D409-06; C07D413-10; C07D417-06; C07D417-10

OS MARPAT 125:114611
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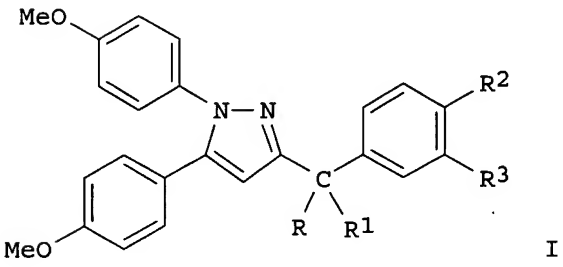

I

AB Pyrazole derivs. I (R = H, OH, OMe, OEt; R1 = H, OMe; RR1 = O, OCH2CH2O, O(CH2)3O; R2 = H, OH, F, Cl, Br, OMe, CF3, CONH2, etc.; R3 = H, F, Cl, OMe, CH2OMe, CO2H, CO2Me, CONH2, etc.) can suppress the production of both prostaglandins and leukotrienes simultaneously, and, therefore, exhibit anti-inflammatory and analgesic effects. Among the approx. 160 compds. prepared, I (R = R1 = OMe, R2 = Cl, Me, R3 = CONH2; R = H, R1 = OMe , R2 = Cl, R3 = CONH2) were claimed.
ST pyrazole antiinflammatory analgesic prepn
IT **Analgesics**
Inflammation inhibitors
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT

(Reactant or reagent); USES (Uses)
(preparation of analgesic and antiinflammatory pyrazole derivs.)

IT 179325-42-9P 179325-44-1P 179325-45-2P 179325-46-3P 179325-47-4P
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179326-66-0P **179326-67-1P** 179326-68-2P 179326-69-3P
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179326-80-8P 179326-81-9P **179326-82-0P** 179326-90-0P
179326-91-1P 179326-92-2P 179326-93-3P 179326-97-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 179325-49-6P 179325-62-3P 179325-65-6P 179325-66-7P 179326-00-2P
179326-14-8P 179326-96-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of analgesic and antiinflammatory pyrazole derivs.)

IT 2592-95-2, 1-Hydroxybenzotriazole 5370-67-2, 2-Dimethoxymethylthiophene
21739-92-4, 2-Chloro-5-bromobenzoic acid 93105-73-8 119517-21-4
119517-96-3, 1,5-Bis(4-methoxyphenyl)-3-pyrazolecarboxaldehyde
179326-59-1 179327-00-5 179327-01-6 **179327-02-7**
179327-03-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of analgesic and antiinflammatory pyrazole derivs.)

IT 179325-42-9P 179325-43-0P 179325-79-2P 179325-85-0P 179325-86-1P
179325-87-2P 179326-72-8P 179326-73-9P 179326-74-0P 179326-75-1P
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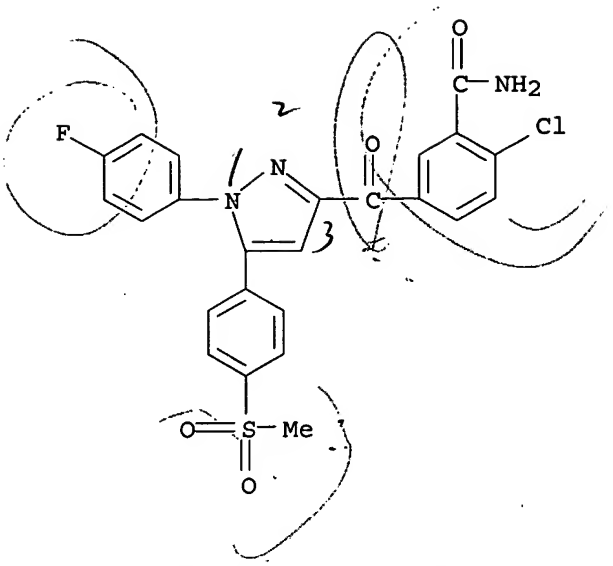
179326-95-5P 179326-98-8P 179326-99-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of analgesic and antiinflammatory pyrazole derivs.)

IT **179325-58-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 179325-58-7 HCAPLUS
CN Benzamide, 2-chloro-5-[[1-(4-fluorophenyl)-5-[4-(methylsulfonyl)phenyl]-1H-pyrazol-3-yl]carbonyl]- (9CI) (CA INDEX NAME)



102 (9)

L102 ANSWER 24 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:410945 HCAPLUS
DN 125:114612
ED Entered STN: 16 Jul 1996
TI Substituted pyrazolylbenzenesulfonamide for the treatment of inflammation
IN **Graneto, Matthew J.**
PA **G.D. Searle** and Co., USA
SO U.S., 24 pp., Cont.-in-part of U.S. Ser. No. 160,594.
CODEN: USXXAM
DT Patent
LA English
IC ICM A61K043-56
ICS C07D231-12
NCL 514406000
CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63
FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5521207	A	19960528	US 1994-223629	19940406 <--
	US 5466823	A	19951114	US 1993-160594	19931130 <--
	CA 2177576	AA	19950608	CA 1994-2177576	19941114 <--
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	WO 9515316	A1	19950608	WO 1994-US12720	19941114 <--
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	RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9511714	A1	19950619	AU 1995-11714	19941114 <--
	AU 690609	B2	19980430		
	EP 731795	A1	19960918	EP 1995-902444	19941114 <--
	EP 731795	B1	19991222		
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	HU 74180	A2	19961128	HU 1996-1455	19941114 <--
	CN 1141630	A	19970129	CN 1994-194833	19941114 <--
	CN 1061036	B	20010124		
	EP 922697	A1	19990616	EP 1999-101687	19941114 <--
	EP 922697	B1	20030226		
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	EP 924201	A1	19990623	EP 1999-101677	19941114 <--

EP	924201	B1	20020206		
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ES	2141916	T3	20000401	ES 1995-902444	19941114 <--
PT	731795	T	20000531	PT 1995-902444	19941114 <--
PL	180717	B1	20010330	PL 1994-314695	19941114 <--
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ZA	9409418	A	19951128	ZA 1994-9418	19941128 <--
US	5504215	A	19960402	US 1995-458079	19950601 <--
US	5508426	A	19960416	US 1995-457185	19950601 <--
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FI	9602249	A	19960529	FI 1996-2249	19960529 <--
NO	9602184	A	19960529	NO 1996-2184	19960529 <--
US	5760068	A	19980602	US 1996-648113	19960906 <--
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CN	1134417	B	20040114		
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US	6586603	B1	20030701	US 2002-274679	20021021 <--
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JP	1999-298879	A3	19941114 <--		
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US	1997-957345	B1	19971024		
US	1999-449076	A1	19991124		
US	2000-609011	A2	20000530		
US	2002-125325	A1	20020417		
US	2002-274679	A1	20021021		
US	2003-378781	A1	20030304		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 5521207	ICM	A61K043-56
	ICS	C07D231-12
	NCL	514406000

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US 6413960 ECLA C07D231/12B3; C07D231/12B5; C07D231/14; C07D231/16; C07D231/54; C07D401/04; C07D403/0; C07D405/04; C07D405/04; C07D405/04; C07D409/04; C07D495/04 <--
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AB A class of pyrazolylbenzenesulfonamide compds. is described for use in treating inflammation and inflammation-related disorders.

ST pyrazolylbenzenesulfonamide prepn antiinflammatory

IT **Inflammation inhibitors**
(pyrazolylbenzenesulfonamides)

IT 75-36-5, Acetyl chloride 88-15-3, 2-Acetylthiophene 92-91-1, 4-Acetylbiphenyl 96-48-0, γ-Butyrolactone 98-86-2, Acetophenone, reactions 99-91-2, 4'-Chloroacetophenone 321-28-8, 2-Fluoroanisole 356-27-4, Ethyl heptafluorobutyrate 364-83-0, 2',4'-Difluoroacetophenone 383-63-1, Ethyl trifluoroacetate 403-42-9 426-65-3, Ethyl pentafluoropropionate 454-31-9, Ethyl difluoroacetate 529-34-0, 1-Tetralone 553-90-2, Dimethyl oxalate 709-63-7, 4'-(Trifluoromethyl)acetophenone 932-66-1, 1-Acetyl-1-cyclohexene 1443-80-7, 4-Acetylbenzonitrile 1514-87-0, Methyl 2-chloro-2,2-difluoroacetate 1565-17-9, 4-(Aminosulfonyl)acetophenone 1778-09-2, 4'-Methylthioacetophenone 2234-16-4 2642-63-9 2746-25-0, 4-Methoxybenzyl bromide 5370-25-2, 2-Acetyl-5-bromothiophene 6310-09-4, 2-Acetyl-5-chlorothiophene 13670-99-0, 2',6'-Difluoroacetophenone 22047-25-2, 2-Acetylpyrazine 27918-19-0, 4-Sulfonamidophenylhydrazine hydrochloride 39910-98-0, 4'-Morpholinoacetophenone
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of pyrazolylbenzenesulfonamides as antiinflammatories)

IT 318-46-7P, 2-Trifluoroacetyl-1-tetralone 455-91-4P, 3'-Fluoro-4'-methoxyacetophenone 18931-60-7P 39757-35-2P, Methyl 4-[4-chlorophenyl]-2,4-dioxobutanoate 56856-73-6P, 3-(4-Chlorophenyl)-3-ketopropionaldehyde 64287-18-9P, 4,4,4-Trifluoro-1-[2,4-difluorophenyl]butane-1,3-dione 76629-94-2P, 4,4-Difluoro-1-[2-thienyl]butane-1,3-dione 94856-21-0P, 4,4,5,5,5-Pentafluoro-1-[4-chlorophenyl]pentane-1,3-dione 134731-37-6P, 4,4-Difluoro-1-[4-(methylthio)phenyl]butane-1,3-dione 164342-68-1P 170570-76-0P, 4,4-Difluoro-1-[4-chlorophenyl]butane-1,3-dione 170570-77-1P 170570-85-1P, 4,4-Difluoro-1-[2-pyrazinyl]butane-1,3-dione **170570-91-9P** 170570-95-3P, N,N-Bis(4-methoxybenzyl)-4-(aminosulfonyl)acetophenone 170570-96-4P 179184-60-2P, 4,4,4-Trifluoro-1-[2,6-difluorophenyl]butane-1,3-dione 179184-61-3P, 4,4,4-Trifluoro-1-[4-cyanophenyl]-butane-1,3-dione 179184-62-4P, 4,4-Difluoro-1-[4-biphenyl]butane-1,3-dione 179184-63-5P 179184-64-6P, 4,4-Difluoro-1-[4-morpholino]butane-1,3-dione 179184-65-7P, 4,4-Difluoro-1-[2-cyclohexenyl]butane-1,3-dione 179184-66-8P 179184-67-9P, 4,4-Difluoro-1-[4-(trifluoromethyl)phenyl]butane-1,3-dione
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of pyrazolylbenzenesulfonamides as antiinflammatories)

IT **169590-41-4P 169590-42-5P 170569-40-1P**
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170569-91-2P 170569-92-3P 170569-93-4P
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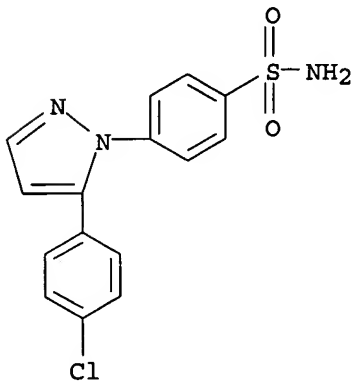
170571-82-1P **170572-13-1P**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation for treating inflammation)

IT **170570-91-9P**
RL: **BAC (Biological activity or effector, except adverse)**; SPN (Synthetic preparation); PREP (Preparation); **THU (Therapeutic use)**
(for preparation of pyrazolylbenzenesulfonamides as antiinflammatories)

RN 170570-91-9 HCAPLUS
CN Benzenesulfonamide, 4-[5-(4-chlorophenyl)-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)



L102 ANSWER 25 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:121332 HCAPLUS
DN 124:289529
ED Entered STN: 28 Feb 1996
TI 3-[4-(Methylsulfonyl)phenyl]-1H-pyrazoles and 4-(1H-pyrazol-3-yl)benzenesulfonamides as selective inhibitors of **cyclooxygenase** II useful as inflammation inhibitors
IN Lee, Len F.; Penning, Thomas D.; Kramer, Steven W.
PA **G. D. Searle** and Co., USA
SO U.S., 40 pp.
CODEN: USXXAM
DT Patent
LA English
IC ICM A61K031-415
ICS C07D231-12
NCL 514406000
CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

FAN.CNT 2

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	EP 772597	A1	19970514	EP 1995-927154	19950720 <--
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	US 5580985	A	19961203	US 1995-535688	19950928 <--
	US 5756530	A	19980526	US 1996-721787	19960925 <--
	US 6028072	A	20000222	US 1997-776090	19970609 <--
PRAI	US 1994-278297	A	19940721 <--		
	EP 1995-927154	A3	19950720 <--		
	WO 1995-US8788	W	19950720 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
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	ICS	C07D231-12
	NCL	514406000

OS MARPAT 124:289529

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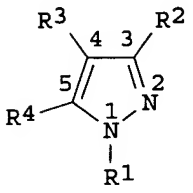

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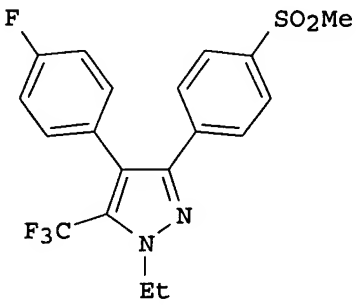

II

AB A class of pyrazolyl compds. is described for use in treating inflammation and inflammation-related disorders and is defined by formula I wherein R1 is a radical selected from hydrido, alkyl, alkenyl, alkynyl, haloalkyl, aralkyl, hydroxyalkyl, alkoxyalkyl, cyanoalkyl, aminoalkyl, alkylaminoalkyl, carboxyalkyl, alkoxycarbonylalkyl, alkylaminocarbonylalkyl, N-hydroxyaminocarbonylalkyl, N-hydroxy-N-alkyl-aminocarbonylalkyl, arylaminocarbonylalkyl and aminocarbonylalkyl; wherein R2 is aryl substituted at a substitutable position with a radical selected from alkylsulfonyl and sulfamyl; wherein R3 is selected from aryl,

cycloalkyl, and cycloalkenyl; wherein R3 is optionally substituted at a substitutable position with one or more radicals selected from halo, alkylthio, alkylsulfinyl, alkyl, cyano, carboxyl, alkoxycarbonyl, aminocarbonyl, alkylaminocarbonyl, arylaminocarbonyl, N-alkyl-N-arylaminocarbonyl, haloalkyl, hydroxyl, alkoxy, hydroxyalkyl, haloalkoxy, amino, alkylamino, arylamino, heterocyclo and nitro; and wherein R4 is selected from hydrido, alkyl, haloalkyl, carboxyalkyl, alkoxycarbonylalkyl, aralkoxycarbonylalkyl, aminocarbonylalkyl, hydroxyalkyl and aralkoxyalkyl; or a pharmaceutically-acceptable salt thereof. Thus, e.g., acylation of thioanisole with 4-fluorophenylacetic acid afforded 2-(4-fluorophenyl)-1-[4-(methylthio)phenyl]ethanone; acylation of the latter with 1-trifluoroacetylimidazole followed by heterocyclization with hydrazine afforded 4-(4-fluorophenyl)-3-[4-(methylthio)phenyl]-5-(trifluoromethyl)-1H-pyrazole; oxidation of latter to the 4-methylsulfonyl derivative followed by 1-ethylation afforded 1-ethyl-4-(4-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-5-(trifluoromethyl)-1H-pyrazole (II) which exhibited selective inhibition of **cyclooxygenase** II: ID50 = >10 μM for COX I, and <0.1 μM for COX II.

ST pyrazole deriv inflammation **cyclooxygenase** II inhibitor; methylsulfonylphenylpyrazole deriv inflammation **cyclooxygenase** II inhibitor; benzenesulfonamide pyrazolyl inflammation **cyclooxygenase** II inhibitor

IT **Inflammation inhibitors**
(3-[4-(methylsulfonyl)phenyl]-1H-pyrazoles and 4-(1H-pyrazol-3-yl)benzenesulfonamides as selective inhibitors of **cyclooxygenase** II useful as inflammation inhibitors)

IT **175676-91-2P 175677-06-2P 175677-08-4P**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(3-[4-(methylsulfonyl)phenyl]-1H-pyrazoles and 4-(1H-pyrazol-3-yl)benzenesulfonamides as selective inhibitors of **cyclooxygenase** II useful as inflammation inhibitors)

IT **175676-92-3P 175676-97-8P 175676-98-9P**
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RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(3-[4-(methylsulfonyl)phenyl]-1H-pyrazoles and 4-(1H-pyrazol-3-yl)benzenesulfonamides as selective inhibitors of **cyclooxygenase** II useful as inflammation inhibitors)

IT 175679-37-5P 175679-38-6P 175679-39-7P
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RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(3-[4-(methylsulfonyl)phenyl]-1H-pyrazoles and 4-(1H-pyrazol-3-yl)benzenesulfonamides as selective inhibitors of **cyclooxygenase** II useful as inflammation inhibitors)

IT **175676-93-4P** 175676-94-5P 175676-96-7P 175677-00-6P
RL: BYP (Byproduct); PREP (Preparation)
(3-[4-(methylsulfonyl)phenyl]-1H-pyrazoles and 4-(1H-pyrazol-3-yl)benzenesulfonamides as selective inhibitors of **cyclooxygenase** II useful as inflammation inhibitors)

IT 62-53-3, Benzenamine, reactions 100-39-0, Benzyl bromide 100-68-5, Thioanisole 103-63-9, 2-Bromoethylbenzene 105-36-2, Ethyl bromoacetate 106-95-6, Allyl bromide, reactions 106-96-7, Propargyl bromide 405-50-5, 4-Fluorophenylacetic acid 4637-24-5, Dimethylformamide dimethylacetal 7250-67-1, N-(2-Chloroethyl)pyrrolidine hydrochloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(3-[4-(methylsulfonyl)phenyl]-1H-pyrazoles and 4-(1H-pyrazol-3-yl)benzenesulfonamides as selective inhibitors of **cyclooxygenase** II useful as inflammation inhibitors)

IT 87483-29-2P, 2-(4-Fluorophenyl)-1-[4-(methylthio)phenyl]ethanone 165252-26-6P 165252-27-7P 175676-88-7P 175676-89-8P **175676-90-1P** 175676-95-6P 175676-99-0P 175677-03-9P **175677-04-0P 175677-11-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(3-[4-(methylsulfonyl)phenyl]-1H-pyrazoles and 4-(1H-pyrazol-3-yl)benzenesulfonamides as selective inhibitors of **cyclooxygenase** II useful as inflammation inhibitors)

IT **39391-18-9, Cyclooxygenase**
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(II; 3-[4-(methylsulfonyl)phenyl]-1H-pyrazoles and 4-(1H-pyrazol-3-yl)benzenesulfonamides as selective inhibitors of **cyclooxygenase** II useful as inflammation inhibitors)

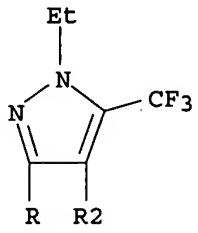
IT **175676-91-2P**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); RCT (Reactant); **THU (Therapeutic use)**; **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

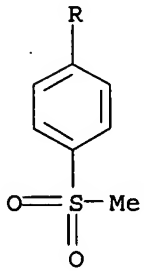
(3-[4-(methylsulfonyl)phenyl]-1H-pyrazoles and 4-(1H-pyrazol-3-yl)benzenesulfonamides as selective inhibitors of **cyclooxygenase** II useful as inflammation inhibitors)

RN 175676-91-2 HCAPLUS

CN 1H-Pyrazole, 1-ethyl-4-(4-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A





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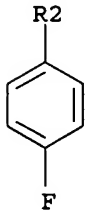

L102 ANSWER 26 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1995:933988 HCAPLUS

DN 123:340111

ED Entered STN: 22 Nov 1995

TI Preparation of 1,5-diphenylpyrazoles for treatment of inflammation and related disorders

IN Lee, Len F.; Bertenshaw, Stephen R.

PA **G.D. Searle** and Co., USA

SO PCT Int. Appl., 31 pp.
CODEN: PIXXD2

DT Patent

LA English

IC ICM C07D231-12
ICS A61K031-415

CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

FAN.CNT 1

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	RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
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	CA 2177824	AA	19950608	CA 1994-2177824	19941114	<--
	AU 9510886	A1	19950619	AU 1995-10886	19941114	<--
	EP 731793	A1	19960918	EP 1995-901778	19941114	<--
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PRAI	US 1993-160553	A	19931130	<--		
	WO 1994-US12718	W	19941114	<--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES	
WO 9515315	ICM	C07D231-12	
	ICS	A61K031-415	
US 5475018	ECLA	A61K031/415; C07D231/12B5	<--

OS MARPAT 123:340111

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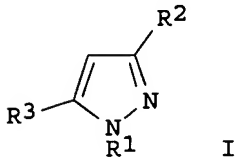

I

AB Title compds. [I; R1 = 4-(alkylsulfonyl)phenyl; R2 = haloalkyl; R3 = (halo)phenyl] were prepared Thus, 4-FC6H4COMe was condensed with CF3CN and the product hydrolized to give 4-FC6H4COCH:C(OH)CF3 which was cyclocondensed with 4-(MeO2S)C6H4NHNH2 to give I [R1 = 4-(MeO2S)C6H4, R2 = CF3, R3 = 4-FC6H4] which gave 38 and 37% inhibition of carrageenan-induced edema and hyperalgesia of rat paw at 10 and 20mg/kg orally, resp.

ST phenylpyrazole prepn antiinflammatory analgesic

IT **Analgesics**
Antipyretics
Inflammation inhibitors
(1,5-diphenylpyrazoles)

IT **Inflammation inhibitors**
(antiarthritics, 1,5-diphenylpyrazoles)

IT **162054-19-5P 170630-30-5P 170630-31-6P**
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170630-53-2P

RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1,5-diphenylpyrazoles for treatment of inflammation and related disorders)

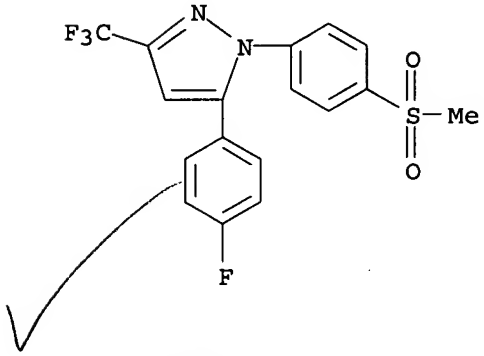
IT 170630-55-4P **170630-56-5P**
RL: BYP (Byproduct); PREP (Preparation)
(preparation of 1,5-diphenylpyrazoles for treatment of inflammation and related disorders)

IT 403-42-9 877-66-7, 4-(Methylsulfonyl)phenylhydrazine
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 1,5-diphenylpyrazoles for treatment of inflammation and related disorders)

IT 170630-54-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1,5-diphenylpyrazoles for treatment of inflammation and related disorders)

IT **162054-19-5P**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1,5-diphenylpyrazoles for treatment of inflammation and related disorders)

RN 162054-19-5 HCAPLUS
CN 1H-Pyrazole, 5-(4-fluorophenyl)-1-[4-(methylsulfonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L102 ANSWER 27 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:931246 HCAPLUS
DN 123:340112
ED Entered STN: 21 Nov 1995
TI Preparation of pyrazolylbenzenesulfonamides as antiinflammatories.
IN **Talley, John J.**; Penning, Thomas D.; Collins, Paul W.; Rogier, Donald J., Jr.; Malecha, James W.; Miyashiro, Julie M.; Bertenshaw, Stephen R.; Khanna, Ish K.; **Granets, Matthew J.**; et al.
PA **G. D. Searle** and Co., USA
SO PCT Int. Appl., 254 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D231-12
ICS A61K031-415; C07D231-14; C07D231-16; C07D231-18; C07D231-54; C07D401-04; C07D403-04; C07D405-04; C07D409-04; C07D495-04
CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 4

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PI	WO 9515316	A1	19950608	WO 1994-US12720	19941114	<--
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	RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
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CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES	
WO 9515316	ICM	C07D231-12	
	ICS	A61K031-415; C07D231-14; C07D231-16; C07D231-18; C07D231-54; C07D401-04; C07D403-04; C07D405-04; C07D409-04; C07D495-04	
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C07D409/04; C07D409/04; C07D495/0; C07D231/12B5;
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C07D405/04; C07D405/04; C07D409/04; C07D495/04 <--

OS MARPAT 123:340112
GI For diagram(s), see printed CA Issue.
AB Title compds. [I; R1 = (substituted) (hetero)aryl; R2 = H, alkyl, haloalkyl, alkoxycarbonyl, cyano, NO2, cyanoalkyl, carboxyl, aminocarbonyl, alkylaminocarbonyl, carboxyalkylaminocarbonyl, carboxyalkyl, aralkoxycarbonylalkylaminocarbonyl, aminocarbonylalkyl, alkoxycarbonylcyanoalkenyl, hydroxyalkyl etc.; R3 = H, alkyl, cyano, NO2, formyl, cyanoamidino, hydroxyalkyl, cycloalkyl, alkylsulfonyl, halo, heterocyclyl, heterocyclylalkyl, etc.; R4 = (substituted) aralkenyl, aryl, cycloalkyl, cycloalkenyl, heterocyclyl; R3R4 = Q1; m = 1-3; A = Ph, 5-6 membered heterocyclyl; R6 = halo, alkylthio, alkylsulfinyl, alkylsulfonyl, cyano, carboxyl, aminocarbonyl, sulfamyl, NO2, acylamino, etc.; provided R2 and R3 do not both = H, carboxy, ethoxycarbonyl; further provided that R2 ≠ carboxyl, Me when R3 = H and when R4 is Ph; further provided that R4 ≠ triazolyl when R2 = Me; further provided that R4 ≠ aralkenyl when R2 = carboxyl, aminocarbonyl, ethoxycarbonyl; further provided that R4 ≠ Ph when R2 = Me and R3 = carboxyl; and further provided that R4 ≠ unsubstituted thienyl when R2 = trifluoromethyl], were prepared Thus, F3CCO2Et in MeOCMe3 was treated with 25% NaOMe and then 4'-chloroacetophenone followed by stirring overnight to give 85% 4,4,4-trifluoro-1-(4-chlorophenyl)butane-1,3-dione. The latter was refluxed with 4-sulfonamidophenylhydrazine hydrochloride in EtOH to give title compound (II). II inhibited human **cyclooxygenase** II and I with ID50 = <.1 μM and 18 μM, resp.
ST pyrazolylbenzenesulfonamide prepn **cyclooxygenase** inhibitor; antiinflammatory pyrazolylbenzenesulfonamide; analgesic pyrazolylbenzenesulfonamide
IT **Analgesics**
(inhibitors of **cyclooxygenase** II; preparation of pyrazolylbenzenesulfonamides as antiinflammatories)
IT **Inflammation inhibitors**
(preparation of pyrazolylbenzenesulfonamides as antiinflammatories)
IT **39391-18-9, Cyclooxygenase**
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(inhibitors of **cyclooxygenase** II; preparation of pyrazolylbenzenesulfonamides as antiinflammatories)
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RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU**

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolylbenzenesulfonamides as antiinflammatories)

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RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolylbenzenesulfonamides as antiinflammatories)

IT 74-88-4, Methyl iodide, reactions 74-95-3, Dibromomethane 75-36-5, Acetyl chloride 77-78-1, Dimethyl sulfate 93-55-0, Propiophenone 96-48-0, γ-Butyrolactone 98-86-2, Acetophenone, reactions 99-91-2, 4'-Chloroacetophenone 100-06-1 100-58-3, Phenylmagnesium bromide 105-56-6, Ethyl cyanoacetate 106-31-0, Butyric anhydride 106-47-8, 4-Chloroaniline, reactions 108-24-7, Acetic anhydride 109-94-4, Ethyl formate 116-54-1, Methyl dichloroacetate 122-00-9, 4'-Methylacetophenone 137-06-4, o-Thiocresol 321-28-8, 2-Fluoroanisole 356-27-4, Ethyl heptafluorobutyrate 383-63-1, Ethyl trifluoroacetate 437-82-1, 2,6-Difluoroanisole 454-31-9, Ethyl difluoroacetate 488-17-5, 3-Methylcatechol 529-34-0, 1-Tetralone 553-90-2, Dimethyl oxalate 578-58-5, 2-Methylanisole 823-85-8, 4-Fluorophenylhydrazine hydrochloride 1132-05-4, 3-Allyl-4-hydroxyacetophenone 1514-87-0, Methyl chlorodifluoroacetate 1546-79-8, 1-Trifluoroacetylimidazole 1565-17-9 1984-65-2, 2,6-Dichloroanisole 2687-43-6, O-Benzylhydroxylamine hydrochloride 2746-25-0, 4-Methoxybenzyl bromide 2892-18-4, 5-Methyl-1-phenyl-1-hexen-3-one 3162-29-6 4653-11-6, 4-(2-Thienyl)butyric acid 7051-34-5, Bromomethylcyclopropane 14804-32-1, 2-Ethylanisole 22047-25-2, Acetylpyrazine 27918-19-0, 4-Sulfonamidophenylhydrazine hydrochloride 51015-29-3, 6-Methyl-1-Tetralone
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrazolylbenzenesulfonamides as antiinflammatories)

IT 318-46-7P 322-06-5P, 4,4,4-Trifluoro-2-methyl-1-phenylbutane-1,3-dione 326-06-7P, 4,4,4-Trifluoro-1-phenylbutane-1,3-dione 403-42-9P, 4'-Fluoroacetophenone 450-95-3P, 2-Fluoroacetophenone 455-91-4P 720-94-5P 2388-73-0P, 2-Methylthioanisole 6542-60-5P, (Cyanomethyl)cyclopropane 6739-22-6P 13414-95-4P 15191-68-1P 18931-60-7P 20487-10-9P 20577-73-5P 23894-54-4P 29643-34-3P 37032-45-4P 39757-34-1P 39757-35-2P 41727-59-7P 56856-73-6P 63301-25-7P 100256-35-7P 106876-38-4P 142499-46-5P 170570-74-8P **170570-75-9P** 170570-76-0P 170570-77-1P 170570-78-2P 170570-79-3P **170570-81-7P** 170570-82-8P **170570-83-9P** 170570-85-1P 170570-86-2P 170570-87-3P **170570-88-4P** 170570-89-5P 170570-90-8P **170570-91-9P** 170570-92-0P **170570-93-1P 170570-94-2P** 170570-95-3P 170570-96-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrazolylbenzenesulfonamides as antiinflammatories)

IT **39391-18-9, Cyclooxygenase**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); MSC (Miscellaneous); **THU**

(Therapeutic use); PROC (Process)
(inhibitors of **cyclooxygenase** II; preparation of pyrazolylbenzenesulfonamides as antiinflammatories)
RN 39391-18-9 HCAPLUS
CN Synthetase, prostaglandin endoperoxide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

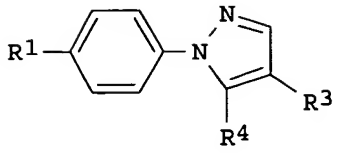
L102 ANSWER 28 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:902660 HCAPLUS
DN 123:313952
ED Entered STN: 08 Nov 1995
TI Preparation of 1,3,5-trisubstituted pyrazoles as antiinflammatories.
IN **Talley, John J.**; Rogier, Donald J., Jr.; Penning, Thomas D.; Yu, Stella S.
PA **G.D. Searle** and Co., USA
SO PCT Int. Appl., 87 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D231-12
ICS C07D405-04; C07D409-04; A61K031-415
CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9515318	A1	19950608	WO 1994-US12722	19941114 <--
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, UZ				
RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5434178	A	19950718	US 1993-160517	19931130 <--
CA 2177574	AA	19950608	CA 1994-2177574	19941114 <--
AU 9511715	A1	19950619	AU 1995-11715	19941114 <--
EP 731796	A1	19960918	EP 1995-902445	19941114 <--
EP 731796	B1	20000802		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 09505830	T2	19970610	JP 1994-515613	19941114 <--
AT 195118	E	20000815	AT 1995-902445	19941114 <--
ES 2150545	T3	20001201	ES 1995-902445	19941114 <--
PT 731796	T	20010131	PT 1995-902445	19941114 <--
US 5908852	A	19990601	US 1996-647911	19960530 <--
GR 3034515	T3	20001229	GR 2000-402205	20000929 <--
PRAI US 1993-160517	A	19931130 <--		
WO 1994-US12722	W	19941114 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 9515318	ICM	C07D231-12
	ICS	C07D405-04; C07D409-04; A61K031-415

OS CASREACT 123:313952; MARPAT 123:313952
GI



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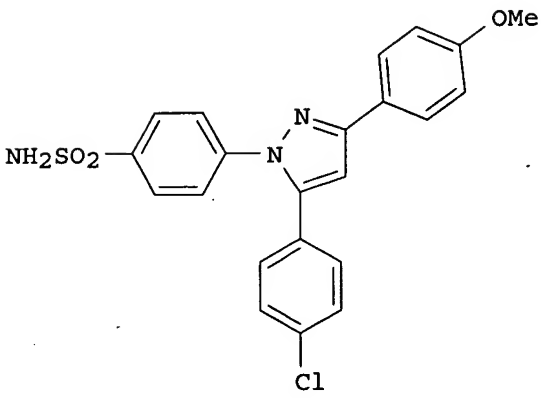

II

AB Title compds. [I; R1 = alkylsulfonyl, sulfamyl; R2, R4 = (substituted) aryl, heterocyclyl; R3 = H, alkyl, haloalkyl, cyano, carboxyl, alkoxycarbonyl, amino, acyl, acylamino, halo, alkylsulfonylamino; provided ≥1 of R2, R4 cannot = Ph or substituted triazole when R1 = sulfamyl; further provided R2 cannot = 4-MeOC6H4 or 4-MeC6H4 when R4 = 4-MeOC6H4 or 4-MeC6H4 and when R1 = sulfamyl; and further provided that R2 cannot = tetrazolyl when R4 = fluorophenyl, and when R1 = MeSO2], were prepared Thus, 4-chloro-4'-methoxychalcone in EtOH/acetone was treated with 30% aqueous H2O2 and 4N NaOH to give 3-(4-chlorophenyl)-2,3-epoxy-4'-methoxypropiophenone. The latter was refluxed with 4-sulfonamidophenylhydrazine hydrochloride in EtOH containing HOAc to give title compound (II). II inhibited **cyclooxygenase** II with ID50 = <0.1 μM.

ST arylpyrazole prepn antiinflammatory; pyrazolylbenzenesulfonamide prepn **cyclooxygenase** inhibitor; pain treatment arylpyrazole

IT **Inflammation inhibitors**
(preparation of 1,3,5-trisubstituted pyrazoles as antiinflammatories)

IT **Analgesics**
(preparation of 1,3,5-trisubstituted pyrazoles as selective **cyclooxygenase** II inhibitors)

IT **Fever and Hyperthermia**
(treatment; preparation of 1,3,5-trisubstituted pyrazoles as selective **cyclooxygenase** II inhibitors)

IT **78794-60-2P 143809-38-5P 143809-39-6P**
169951-22-8P 169951-23-9P 169951-24-0P
169951-25-1P 169951-26-2P 169951-27-3P
169951-28-4P 169951-29-5P 169951-30-8P
169951-31-9P 169951-32-0P 169951-33-1P
169951-34-2P 169951-35-3P 169951-36-4P
169951-37-5P 169951-38-6P 169951-39-7P
169951-40-0P 169951-41-1P 169951-42-2P
169951-43-3P 169951-44-4P 169951-45-5P
169951-46-6P 169951-47-7P 169951-48-8P
169951-49-9P 169951-50-2P 169951-51-3P
169951-52-4P 169951-53-5P 169951-54-6P
169951-55-7P 169951-56-8P 169951-57-9P
169951-58-0P 169951-59-1P 169951-60-4P

169951-61-5P 169951-62-6P 169951-63-7P
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169951-67-1P 169951-68-2P 169951-69-3P
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169951-73-9P 169951-74-0P 169951-75-1P
169951-76-2P 169951-77-3P 169951-78-4P
169951-79-5P 169951-80-8P 169951-81-9P
169951-82-0P 169951-83-1P 169951-84-2P
169951-85-3P 169951-86-4P 169951-87-5P
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169951-94-4P 169951-95-5P 169951-96-6P
169951-97-7P 169951-98-8P 169951-99-9P
169952-00-5P 169952-01-6P 169952-02-7P
169952-03-8P 169952-04-9P 169952-05-0P
169952-06-1P 169952-07-2P 169952-08-3P
169952-09-4P 169952-10-7P 169952-11-8P
169952-12-9P 169952-13-0P
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1,3,5-trisubstituted pyrazoles as antiinflammatories)

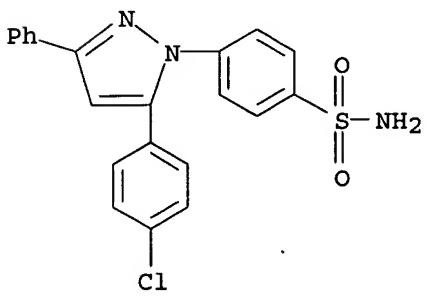
IT 99-91-2, 4'-Chloroacetophenone 120-46-7, Dibenzoylmethane 1126-46-1, Methyl 4-chlorobenzoate 6552-68-7, 4-Chloro-4'-methoxychalcone 17852-67-4, 4-Methylsulfonylphenylhydrazine hydrochloride 27918-19-0, 4-Sulfonamidophenylhydrazine hydrochloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 1,3,5-trisubstituted pyrazoles as antiinflammatories)

IT 18362-49-7P 27547-08-6P **78794-55-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1,3,5-trisubstituted pyrazoles as antiinflammatories)

IT **39391-18-9, Cyclooxygenase**
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(selective inhibitors of **cyclooxygenase** II; preparation of 1,3,5-trisubstituted pyrazoles as antiinflammatories)

IT **78794-60-2P**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1,3,5-trisubstituted pyrazoles as antiinflammatories)

RN 78794-60-2 HCAPLUS
CN Benzenesulfonamide, 4-[5-(4-chlorophenyl)-3-phenyl-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)



L102 ANSWER 29 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN

AN **1995:790898** HCAPLUS
DN **123:217724**
ED Entered STN: 14 Sep 1995
TI Antiinflammatory 4,5-Diarylpyrroles. 2. Activity as a Function of **Cyclooxygenase-2** Inhibition
AU Wilkerson, Wendell Wilkie; Copeland, Robert A.; Covington, Maryanne; Trzaskos, James M.
CS DuPont Merck Pharmaceutical Company, Wilmington, DE, 19880-0353, USA
SO Journal of Medicinal Chemistry (**1995**), 38(20), 3895-901
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
CC 1-3 (Pharmacology)
AB The antiinflammatory activity of a series of 2-substituted- and 2,3-disubstituted-4-(4-fluorophenyl)-5-[4-(methylsulfonyl)phenyl]-1H-pyrroles was previously shown by quant. structure-activity relationship (QSAR) studies to be correlated with the molar refractivity and inductive field effect of the 2-substituent and the lipophilicity of the 3-substituent. The present study demonstrates that much of the antiinflammatory activity of these pyrroles could be correlated with the inhibition of the inducible isoform of **cyclooxygenase** (**COX2**). Addnl. QSAR studies have been used to identify the mol. parameters necessary for maximizing **COX2** inhibition while simultaneously minimizing the inhibition of constitutively expressed **cyclooxygenase-1**. Such an effort should facilitate the discovery and development of selective COX inhibitors that should lead to safer nonsteroidal antiinflammatory drugs.
ST pyrrole aryl antiinflammatory **cyclooxygenase** inhibitor
IT Quantitative structure-activity relationship
(antiinflammatory diarylpyrroles: activity as a function of **cyclooxygenase-2** inhibition)
IT Molecular structure-biological activity relationship
(**cyclooxygenase-2** inhibiting; antiinflammatory diarylpyrroles: activity as a function of **cyclooxygenase-2** inhibition)
IT **Inflammation inhibitors**
(nonsteroid; antiinflammatory diarylpyrroles: activity as a function of **cyclooxygenase-2** inhibition)
IT Molecular structure-biological activity relationship
(inflammation-inhibiting, antiinflammatory diarylpyrroles: activity as a function of **cyclooxygenase-2** inhibition)
IT **39391-18-9**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(2-, inhibitors; antiinflammatory diarylpyrroles: activity as a function of **cyclooxygenase-2** inhibition)
IT **78495-23-5 94985-10-1 94985-11-2 106315-66-6 108381-60-8 108381-61-9**, 1H-Pyrrole, 5-bromo-3-(4-fluorophenyl)-2-[4-(methylsulfonyl)phenyl]- **108381-62-0**, 1H-Pyrrole, 5-chloro-3-(4-fluorophenyl)-2-[4-(methylsulfonyl)phenyl]- **108381-63-1 108381-64-2 108381-65-3**, 1H-Pyrrole, 3-(4-fluorophenyl)-1-methyl-2-[4-(methylsulfonyl)phenyl]- **108381-67-5 108381-68-6 108381-69-7 108400-79-9 153506-55-9 153506-56-0**, 1H-Pyrrole, 3-(4-fluorophenyl)-5-methylsulfonyl-2-[4-methylsulfonyl)phenyl]- **153506-57-1**, 1H-Pyrrole, 3-(4-fluorophenyl)-2-[4-(methylsulfonyl)phenyl]-5-nitro- **153506-58-2 153506-60-6 153506-61-7**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); BIOL (Biological study)
(antiinflammatory diarylpyrroles: activity as a function of **cyclooxygenase-2** inhibition)

IT **39391-18-9**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); BIOL (Biological study)
(2-, inhibitors; antiinflammatory diarylpyrroles: activity as a function of **cyclooxygenase-2** inhibition)
RN 39391-18-9 HCAPLUS
CN Synthetase, prostaglandin endoperoxide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L102 ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:696007 HCAPLUS
DN 123:83360
ED Entered STN: 25 Jul 1995
TI 1,4,5-Triphenyl pyrazolyl compounds for the treatment of inflammation and inflammation-related disorders
IN Lee, Len F.
PA **G.D. Searle** and Co., USA
SO U.S., 14 pp.
CODEN: USXXAM
DT Patent
LA English
IC ICM A61K031-415
ICS C07D231-12; C07D231-14
NCL 548406000
CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	US 5401765	A	19950328	US 1993-161004	19931130	<--
	WO 9515317	A1	19950608	WO 1994-US12721	19941114	<--
	W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, UZ					
	RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
	CA 2177573	AA	19950608	CA 1994-2177573	19941114	<--
	AU 9510887	A1	19950619	AU 1995-10887	19941114	<--
	EP 731794	A1	19960918	EP 1995-901779	19941114	<--
	EP 731794	B1	19970806			
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE					
	JP 09505829	T2	19970610	JP 1994-515612	19941114	<--
	AT 156482	E	19970815	AT 1995-901779	19941114	<--
	ES 2105874	T3	19971016	ES 1995-901779	19941114	<--
	US 5639777	A	19970617	US 1996-648118	19960521	<--
PRAI	US 1993-161004		19931130	<--		
	WO 1994-US12721		19941114	<--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 5401765	ICM	A61K031-415
	ICS	C07D231-12; C07D231-14
	NCL	548406000

OS MARPAT 123:83360
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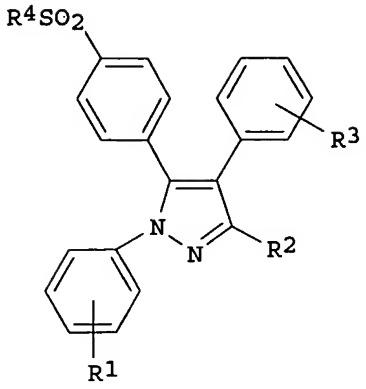

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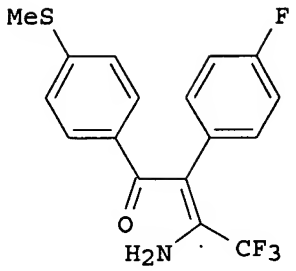


II

AB Compds. of formula I wherein R1 is one or more radicals independently selected from the group hydrido, halo, alkyl, alkylthio, alkylsulfinyl, alkylsulfonyl, nitro, amino, N-monoalkylamino, N,N-dialkylamino, acylamino, acylaminoalkyl, haloalkyl, hydroxy and alkoxy; wherein R2 is selected from hydrido, alkyl, cyano and haloalkyl; wherein R3 is one or more radicals independently selected from the group hydrido, halo, alkyl, alkylthio, alkylsulfinyl, alkylsulfonyl, nitro, amino, N-monoalkylamino, N,N-dialkylamino, acylamino, acylaminoalkyl, haloalkyl, hydroxy and alkoxy; and wherein R4 is alkyl; or a pharmaceutically-acceptable salt thereof useful for the treatment of inflammation, including treatment of pain and disorders such as arthritis. Thus, e.g., treatment of 2-(4-fluorophenyl)-1-[4-(methylthio)phenyl]ethanone with NaH/DMF followed by gaseous trifluoroacetonitrile afforded 3-amino-4,4,4-trifluoro-2-(4-fluorophenyl)-1-[4-(methylthio)phenyl]-2-buten-1-one (II); hydrolysis of enamine II to the diketone, followed by cyclocondensation with phenylhydrazine afforded a mixture containing the desired 4-(4-fluorophenyl)-5-[4-(methylthio)phenyl]-1-phenyl-3-(trifluoromethyl)pyrazole together with its regioisomer 4-(4-fluorophenyl)-3-[4-(methylthio)phenyl]-1-phenyl-5-(trifluoromethyl)pyrazole (HPLC purifn); oxidation of the desired isomer with H2O2 afforded I (R4 = Me, R3 = 4-F, R2 = CF3, R1 = H) which displayed 20% inhibition of rat carrageenan foot pad edema @ 10 mg/kg body weight

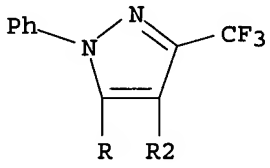
ST inflammation inhibitor triphenylpyrazolyl deriv; phenylpyrazole tri deriv antiinflammatory; pyrazole triphenyl deriv antiinflammatory

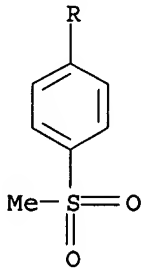
IT **Inflammation inhibitors**
(1,4,5-tri-Ph pyrazolyl compds. for the treatment of inflammation and inflammation-related disorders)

IT **165251-89-8P 165251-90-1P 165251-91-2P**
165251-92-3P 165251-93-4P 165251-94-5P
165251-95-6P 165251-96-7P 165251-97-8P
165251-98-9P 165251-99-0P 165252-00-6P
165252-01-7P 165252-02-8P 165252-03-9P
165252-04-0P 165252-05-1P 165252-06-2P
165252-07-3P 165252-08-4P 165252-09-5P
165252-10-8P 165252-11-9P 165252-12-0P
165252-13-1P 165252-14-2P 165252-15-3P
165252-16-4P 165252-17-5P 165252-18-6P
165252-19-7P 165252-20-0P 165252-21-1P
165252-22-2P 165252-23-3P 165252-24-4P
165252-25-5P
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(1,4,5-tri-Ph pyrazolyl compds. for the treatment of inflammation and inflammation-related disorders)

IT 165252-29-9P
RL: BYP (Byproduct); PREP (Preparation)
(1,4,5-tri-Ph pyrazolyl compds. for the treatment of inflammation and inflammation-related disorders)
IT 100-63-0, Phenylhydrazine 87483-29-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(1,4,5-tri-Ph pyrazolyl compds. for the treatment of inflammation and inflammation-related disorders)
IT 165252-26-6P 165252-27-7P 165252-28-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(1,4,5-tri-Ph pyrazolyl compds. for the treatment of inflammation and inflammation-related disorders)
IT **165251-89-8P**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(1,4,5-tri-Ph pyrazolyl compds. for the treatment of inflammation and inflammation-related disorders)
RN 165251-89-8 HCAPLUS
CN 1H-Pyrazole, 4-(4-fluorophenyl)-5-[4-(methylsulfonyl)phenyl]-1-phenyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A





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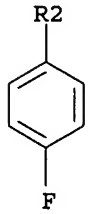


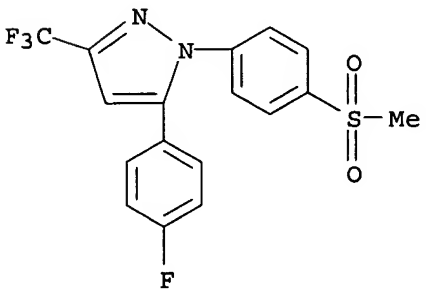
L102 ANSWER 31 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN **1995:631975** HCAPLUS

DN **123:74204**
ED Entered STN: 22 Jun 1995
TI **Cyclooxygenase-2** inhibitory 2-substituted-4,5-diarylpyrroles
AU Wilkerson, Wendell W.; Copeland, Robert A.; Covington, Maryanne B.; Grubb, Mary F.; Hewes, Walter E.; Kerr, Janet S.; Trzaskos, James M.
CS DuPont Merck Pharmaceutical Company, Wilmington, DE, 19880-0353, USA
SO Medicinal Chemistry Research (**1995**), 5(5), 399-408
CODEN: MCREEB; ISSN: 1054-2523
PB Birkhaeuser
DT Journal
LA English
CC 1-3 (Pharmacology)
AB Twenty 2-substituted-4-(4-substituted phenyl)-5-(4-substituted phenyl)-1H-pyrroles were assayed for their ability to inhibit **cyclooxygenase-2** (**COX-2**) and exhibit systemic antiinflammatory activity in the rat established adjuvant arthritis model. Quant. structure-activity (QSAR) studies were used in an attempt to understand the observed correlation between oral activity and **COX2** inhibition.
ST QSAR diarylpyrrole **cyclooxygenase** inhibitor antiinflammatory
IT **Inflammation inhibitors**
(2-substituted-4,5-diarylpyrroles)
IT Quantitative structure-activity relationship
(of **cyclooxygenase-2** inhibitory 2-substituted-4,5-diarylpyrroles)
IT **Inflammation inhibitors**
(**antiarthritics**, **Cyclooxygenase-2** inhibitory 2-substituted-4,5-diarylpyrroles)
IT **39391-18-9**, **Cyclooxygenase**
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(**2**; QSAR of antiinflammatory and **cyclooxygenase 2**-inhibitory diarylpyrroles)
IT 73800-00-7 **78495-23-5** **78495-38-2** 94985-08-7 **94985-10-1** **94985-11-2** 95013-72-2 **106315-66-6** **108381-61-9** **108381-62-0** **108381-63-1** **153506-55-9** **153506-56-0** **153506-57-1** **165328-54-1** 165328-55-2 **165328-56-3** 165328-57-4 165328-58-5 **165328-59-6**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); PRP (Properties); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(QSAR of antiinflammatory and **cyclooxygenase 2**-inhibitory diarylpyrroles)
IT **39391-18-9**, **Cyclooxygenase**
RL: **BAC (Biological activity or effector, except adverse)**; BIOL (Biological study); **THU (Therapeutic use)**
(**2**; QSAR of antiinflammatory and **cyclooxygenase 2**-inhibitory diarylpyrroles)
RN 39391-18-9 HCAPLUS
CN Synthetase, prostaglandin endoperoxide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L102 ANSWER 32 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN **1995:623853** HCAPLUS
DN **123:101766**
ED Entered STN: 21 Jun 1995
TI Mediation of inflammation by **cyclooxygenase-2**
AU Seibert, Karen; Masferrer, Jaime; Zhang, Yan; Gregory, Susan; Olson, Gary; Hauser, Scott; Leahy, Kathleen; Perkins, William; Isakson, Peter
CS Inflammatory Disease Research, St. Louis, MO, 63167, USA
SO Agents and Actions Supplements (**1995**), 46, 41-50

CODEN: AASUDJ; ISSN: 0379-0363
DT Journal; General Review
LA English
CC 1-0 (Pharmacology)
AB A review with 20 refs. Non-steroidal antiinflammatory drugs (NSAIDs) are commonly used for the treatment of inflammation, pain, and fever. Mechanistically, these compds. are believed to act via inhibition of the enzyme **cyclooxygenase** (COX), which catalyzes the conversion of arachidonic acid to the prostaglandins (PGs). Although com. available NSAIDS are efficacious antiinflammatory agents, significant side effects limit their use. Recently two forms of COX were identified- a constitutively expressed **COX-1** and a cytokine-inducible **COX-2**. Com. available NSAIDs like indomethacin inhibit both **COX-1** and **COX-2** suggesting the hypothesis that toxicities associated with NSAID therapy are due to inhibition of the non-regulated or constitutive form of COX (**COX-1**) in normal tissues, whereas therapeutic benefit derives from inhibition of the inducible enzyme, **COX-2**, at the site of inflammation. Therefore, a selective inhibitor of **COX-2** may be anti-inflammatory without GI toxicity - providing a significant improvement over currently available NSAIDs.
ST antiinflammatory **cyclooxygenase** inhibitor review
IT **Inflammation**
Inflammation inhibitors
(mediation of inflammation by **cyclooxygenase-2** and pharmacol. of SC-58125)
IT **162054-19-5**, SC 58125
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(mediation of inflammation by **cyclooxygenase-2** and pharmacol. of SC-58125)
IT **39391-18-9**
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(mediation of inflammation by **cyclooxygenase-2** and pharmacol. of SC-58125)
IT **162054-19-5**, SC 58125
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(mediation of inflammation by **cyclooxygenase-2** and pharmacol. of SC-58125)
RN 162054-19-5 HCAPLUS
CN 1H-Pyrazole, 5-(4-fluorophenyl)-1-[4-(methylsulfonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L102 ANSWER 33 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:570840 HCAPLUS
DN 122:314540

ED Entered STN: 25 May 1995
TI Preparation of substituted (4-sulfonylphenyl)oxazoles as inflammation inhibitors
IN **Norman, Bryan H.**; Lee, Len F.; Masferrer, Jaime L.; **Talley, John J.**
PA **G.D. Searle** and Co., USA
SO PCT Int. Appl., 193 pp.
CODEN: PIXXD2
DT Patent
LA English
IC C07D263-32
CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 25

FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9427980	A1	19941208	WO 1994-US5395	19940519 <--
	W: AT, AU, BB, BG, BR, CA, CH, CN, CZ, DE, DK, ES, FI, GB, HU, JP, KR, LU, NL, NO, NZ, PL, PT, RO				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, NL, PT, SE				
	US 5380738	A	19950110	US 1993-65730	19930521 <--
	CA 2161769	AA	19941208	CA 1994-2161769	19940519 <--
	AU 9469495	A1	19941220	AU 1994-69495	19940519 <--
	EP 699192	A1	19960306	EP 1994-917983	19940519 <--
	EP 699192	B1	20020724		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
	JP 08510736	T2	19961112	JP 1994-500726	19940519 <--
	AT 221054	E	20020815	AT 1994-917983	19940519 <--
	PT 699192	T	20021231	PT 1994-917983	19940519 <--
	ES 2180580	T3	20030216	ES 1994-917983	19940519 <--
	US 5719163	A	19980217	US 1995-535227	19951027 <--
	US 6090834	A	20000718	US 1998-203451	19981201 <--
PRAI	US 1993-65730	A	19930521 <--		
	WO 1994-US5395	W	19940519 <--		
	US 1995-445312	A1	19950519 <--		
	US 1998-12665	B1	19980123		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 9427980	IC	C07D263-32

OS MARPAT 122:314540
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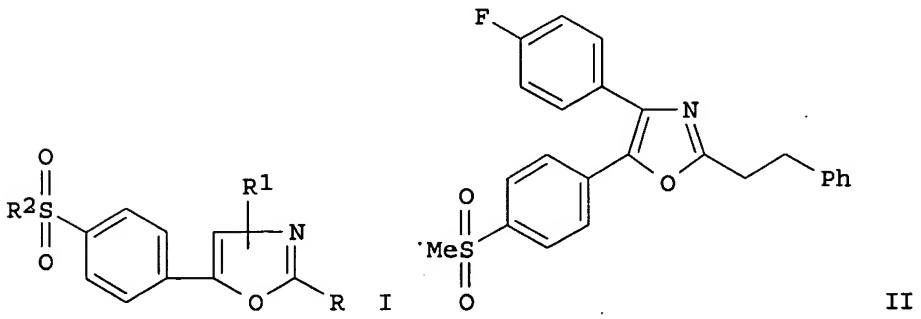

AB The title compds., (4-sulfonylphenyl)oxazoles I (R = H, alkyl, hydroxyalkyl, etc.; R1 = cycloalkyl, cycloalkenyl, etc.; R2 = alkyl, haloalkyl, amino) were disclosed as inflammation inhibitors. An example compound, 4-(4-fluorophenyl)-5-[4-(methylsulfonyl)phenyl]-2-(2-phenylethyl)oxazole (II) was prepared

ST oxazole sulfonylphenyl prepn inflammation inhibitor

IT **Analgesics**
Inflammation inhibitors
(preparation of (sulfonylphenyl)oxazoles)

IT 108-43-0, 3-Chlorophenol 405-50-5, 4-Fluorophenylacetic acid 645-45-4, Hydrocinnamoyl chloride 2043-61-0, Cyclohexanecarboxaldehyde 3446-89-7, 4-(Methylthio)benzaldehyde 16311-69-6, 3,4-Dimethyl-5-(2-hydroxyethyl)thiazolium iodide 36187-57-2 163303-23-9 163304-90-3 163304-91-4 163304-96-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of (sulfonylphenyl)oxazoles as inflammation inhibitors)

IT 71006-38-7P 157671-95-9P 163303-20-6P 163303-21-7P 163303-22-8P 163303-24-0P 163304-92-5P 163304-93-6P 163304-94-7P 163304-95-8P 163304-97-0P 163304-98-1P 163304-99-2P **163305-00-8P** 163305-01-9P 163305-02-0P 163305-03-1P 163305-04-2P 163305-05-3P 163305-06-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (sulfonylphenyl)oxazoles as inflammation inhibitors)

IT **163303-33-1P 163303-34-2P 163303-35-3P 163303-37-5P 163303-46-6P 163303-48-8P 163303-50-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of (sulfonylphenyl)oxazoles as inflammation inhibitors)

IT **163303-18-2P 163303-19-3P 163303-25-1P 163303-26-2P 163303-27-3P 163303-28-4P 163303-29-5P 163303-30-8P 163303-31-9P 163303-32-0P 163303-36-4P 163303-38-6P 163303-39-7P 163303-40-0P 163303-41-1P 163303-42-2P 163303-43-3P 163303-44-4P 163303-45-5P 163303-47-7P 163303-49-9P 163303-51-3P 163303-52-4P 163303-53-5P 163303-54-6P 163303-55-7P 163303-56-8P 163303-57-9P 163303-58-0P 163303-59-1P 163303-60-4P 163303-61-5P 163303-62-6P 163303-63-7P 163303-64-8P 163303-65-9P 163303-66-0P 163303-67-1P 163303-68-2P 163303-69-3P 163303-70-6P 163303-71-7P 163303-72-8P 163303-73-9P 163303-74-0P 163303-75-1P 163303-76-2P 163303-77-3P 163303-78-4P 163303-79-5P 163303-80-8P 163303-81-9P 163303-82-0P 163303-83-1P 163303-84-2P 163303-85-3P 163303-86-4P 163303-87-5P 163303-88-6P 163303-89-7P 163303-90-0P 163303-91-1P 163303-92-2P 163303-93-3P 163303-94-4P 163303-95-5P 163303-96-6P 163303-97-7P 163303-98-8P 163303-99-9P 163304-00-5P 163304-01-6P 163304-02-7P 163304-03-8P 163304-04-9P 163304-05-0P 163304-06-1P 163304-07-2P 163304-08-3P 163304-09-4P 163304-10-7P 163304-11-8P 163304-12-9P 163304-13-0P 163304-14-1P 163304-15-2P 163304-16-3P 163304-17-4P 163304-18-5P 163304-19-6P 163304-20-9P 163304-21-0P 163304-22-1P 163304-23-2P 163304-24-3P 163304-25-4P 163304-26-5P 163304-27-6P 163304-28-7P 163304-29-8P 163304-30-1P 163304-31-2P 163304-32-3P 163304-33-4P 163304-34-5P 163304-35-6P 163304-36-7P 163304-37-8P 163304-38-9P 163304-39-0P 163304-40-3P**

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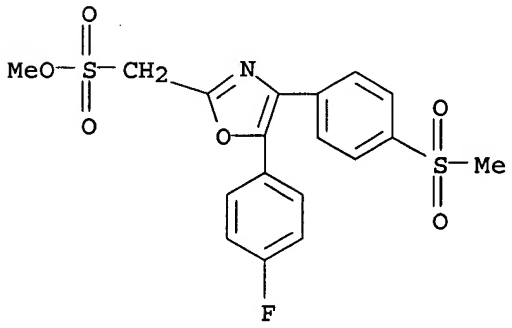
163304-86-7P 163304-87-8P 163304-88-9P
163304-89-0P
RL: SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of (sulfonylphenyl)oxazoles as inflammation inhibitors)

IT **163305-00-8P**
RL: RCT (Reactant); **THU (Therapeutic use)**; **THU (Therapeutic use)**; RACT (Reactant or reagent)
(preparation of (sulfonylphenyl)oxazoles as inflammation inhibitors)

RN 163305-00-8 HCAPLUS
CN 2-Oxazolemethanesulfonic acid, 5-(4-fluorophenyl)-4-[4-(methylsulfonyl)phenyl]-, methyl ester (9CI) (CA INDEX NAME)



L102 ANSWER 34 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN **1995:417224** HCAPLUS
DN **122:204731**
ED Entered STN: 16 Mar 1995
TI Discovery of a better aspirin
AU Isakson, Peter; Seibert, Karen; Masferrer, Jaime; Salvemini, Daniela; Lee, Len; Needleman, Philip
CS Inflammatory Diseases Research, **G.D. Searle** and Monsanto Corporate Research, St. Louis, MO, 63198, USA
SO Advances in Prostaglandin, Thromboxane, and Leukotriene Research (**1995**), 23(Prostaglandins and Related Compounds), 49-54
CODEN: ATLRD6; ISSN: 0732-8141
DT Journal
LA English
CC 1-7 (Pharmacology)
AB The authors showed that a highly selective inhibitor of the **cyclooxygenase** isomer **COX-2** is anti-inflammatory in vivo without causing gastric lesions, while traditional nonsteroidal anti-inflammatory drugs like indomethacin are

both anti-inflammatory and ulcerogenic, consistent with their ability to inhibit **cyclooxygenase COX-1** as well as **COX-2**. Development of selective **COX-2** inhibitors that spare gastric prostaglandin production may represent a significant advance for the treatment of acute and chronic inflammatory disorders.

ST **cyclooxygenase** inhibitor nonsteroidal antiinflammatory drug ulcerogenic

IT **Inflammation inhibitors**
Ulcer
(**cyclooxygenase COX-2** inhibitors as **nonsteroidal** anti-inflammatory drugs without ulcerogenic activity)

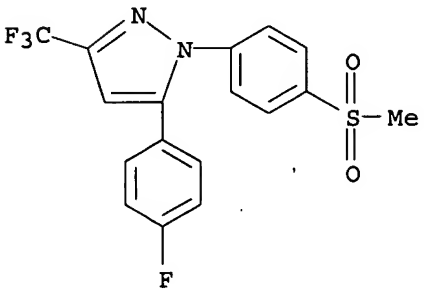
IT 53-86-1, Indomethacin 88149-94-4, DuP 697 123653-11-2, NS 398 **162054-19-5**, SC 58125
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(**cyclooxygenase COX-2** inhibitors as nonsteroidal anti-inflammatory drugs without ulcerogenic activity)

IT **39391-18-9**, **Cyclooxygenase**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(**cyclooxygenase COX-2** inhibitors as nonsteroidal anti-inflammatory drugs without ulcerogenic activity)

IT **162054-19-5**, SC 58125
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(**cyclooxygenase COX-2** inhibitors as nonsteroidal anti-inflammatory drugs without ulcerogenic activity)

RN 162054-19-5 HCAPLUS

CN 1H-Pyrazole, 5-(4-fluorophenyl)-1-[4-(methylsulfonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L102 ANSWER 35 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN

AN **1994:8589** HCAPLUS

DN **120:8589**

ED Entered STN: 08 Jan 1994

TI Preparation of pyrazole derivatives with antiinflammatory, analgesic, and antithrombolic activity

IN Matsuo, Masaaki; Tsuji, Kiyoshi; Ogino, Takashi; Konishi, Nobukiyo

PA Fujisawa Pharmaceutical Co., Ltd., Japan

SO Eur. Pat. Appl., 40 pp.
CODEN: EPXXDW

DT Patent

LA English

IC ICM C07D231-12
ICS C07D231-16; C07D405-04; C07D231-14; A61K031-415

CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	EP 554829	A2	19930811	EP 1993-101569	19930202	<--
	EP 554829	A3	19940608			
	EP 554829	B1	20020515			
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE					
	IL 104311	A1	19970713	IL 1993-104311	19930105	<--
	ZA 9300077	A	19930804	ZA 1993-77	19930106	<--
	JP 05246997	A2	19930924	JP 1993-10379	19930126	<--
	AU 9332174	A1	19930812	AU 1993-32174	19930202	<--
	AU 663149	B2	19950928			
	AT 217613	E	20020615	AT 1993-101569	19930202	<--
	ES 2173875	T3	20021101	ES 1993-101569	19930202	<--
	CA 2088835	AA	19930806	CA 1993-2088835	19930204	<--
	CN 1075959	A	19930908	CN 1993-101069	19930204	<--
	CN 1045767	B	19991020			
	RU 2128172	C1	19990327	RU 1993-4484	19930204	<--
	HU 63392	A2	19930830	HU 1993-309	19930205	<--
	US 5550147	A	19960827	US 1995-413939	19950330	<--
	US 5670533	A	19970923	US 1995-579974	19951228	<--
PRAI	GB 1992-2442	A	19920205	<--		
	GB 1992-20427	A	19920928	<--		
	US 1993-297	B1	19930104	<--		
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CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
EP 554829	ICM	C07D231-12
	ICS	C07D231-16; C07D405-04; C07D231-14; A61K031-415

OS MARPAT 120:8589

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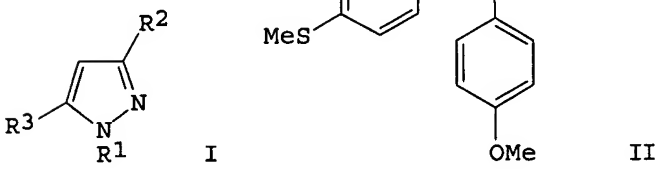

AB Title compds. (I; R1 = substituted aryl; R2 = halo, haloalkyl, cyano, acyl; R3 = substituted aryl) were prepared Thus, 4-(MeS)C6H4COCH2COCHF2 was cyclocondensed with 4-(MeO)C6H4NHNH2·HCl to give title compound II which gave 93.6% inhibition of mycobacterial adjuvant-induced secondary lesion in rats receiving 3.2 mg/kg/day orally for 23 days.

ST pyrazole prepn antiinflammatory analgesic antithrombotic

IT **Analgesics**
Anticoagulants and Antithrombotics
Inflammation inhibitors
(pyrazole derivs.)

IT Autoimmune disease
(treatment of, pyrazole derivs. for)

IT Connective tissue

(disease, treatment of, pyrazole derivs. for)
IT Immunity
(disorder, treatment of, pyrazole derivs. for)
IT 151506-38-6P 151506-39-7P 151506-40-0P 151506-41-1P 151506-42-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of antiinflammatory analgesic, and
antithrombotic)
IT 151506-43-3P 151506-44-4P **151506-45-5P** 151506-46-6P
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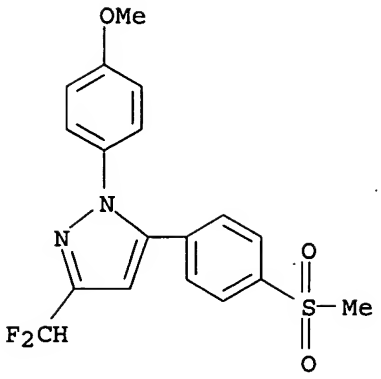
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as antiinflammatory, analgesic, and antithrombotic)
IT 2863-98-1, 4-Cyanophenylhydrazine hydrochloride 19501-58-7,
4-Methoxyphenylhydrazine hydrochloride 134729-31-0 134731-32-1
134731-37-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of antiinflammatory, analgesic, and antithrombotic)
IT **151506-45-5P**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as antiinflammatory, analgesic, and antithrombotic)
RN 151506-45-5 HCAPLUS
CN 1H-Pyrazole, 3-(difluoromethyl)-1-(4-methoxyphenyl)-5-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



L102 ANSWER 36 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN **1991:471593** HCAPLUS
DN **115:71593**
ED Entered STN: 23 Aug 1991
TI Preparation of pyrazole derivatives having antiinflammatory, analgesic, and antithrombotic activities
IN Matsuo, Masaaki; Tsuji, Kiyoshi; Konishi, Nobukiyo; Nakamura, Katsuya
PA Fujisawa Pharmaceutical Co., Ltd., Japan
SO Eur. Pat. Appl., 71 pp.
CODEN: EPXXDW
DT Patent
LA English
IC ICM C07D231-14
ICS A61K031-415; C07D231-12; C07D409-04; C07D401-04; C07D403-04; A61K031-38; A61K031-44
CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 1

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PI	EP 418845	A1	19910327	EP 1990-117983	19900919 <--
	EP 418845	B1	19950809		
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	ZA 9007282	A	19910731	ZA 1990-7282	19900912 <--
	IL 95675	A1	19960331	IL 1990-95675	19900913 <--
	US 5134142	A	19920728	US 1990-582358	19900914 <--
	CA 2025599	AA	19910323	CA 1990-2025599	19900918 <--
	CA 2025599	C	20011120		
	HU 57733	A2	19911230	HU 1990-5970	19900919 <--
	HU 208122	B	19930830		
	ES 2088933	T3	19961001	ES 1990-117983	19900919 <--
	JP 03141261	A2	19910617	JP 1990-252319	19900920 <--
	JP 2586713	B2	19970305		
	NO 9004134	A	19910325	NO 1990-4134	19900921 <--
	CN 1050382	A	19910403	CN 1990-107130	19900921 <--
	CN 1046506	B	19991117		
	AU 9063072	A1	19910418	AU 1990-63072	19900921 <--
	AU 637142	B2	19930520		
	RU 2021990	C1	19941030	RU 1990-4831230	19900921 <--
	RU 2059622	C1	19960510	RU 1991-5010250	19911202 <--
PRAI	GB 1989-21466	A	19890922 <--		
	GB 1990-8399	A	19900412 <--		

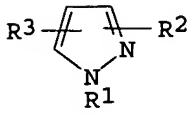
CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
EP 418845	ICM	C07D231-14

ICS A61K031-415; C07D231-12; C07D409-04; C07D401-04; C07D403-04; A61K031-38; A61K031-44

OS MARPAT 115:71593

GI



I

AB The title compds. [I; R1 = heterocyclyl, (un)substituted aryl; R2 = H, CH2NH2, alkylaminomethyl, halomethyl, acyloxymethyl, acyl, acylamino, cyano, halo, alkylthio, alkylsulfinyl; R3 = (un)substituted aryl or heterocyclyl; provided that, e.g. when R2 = (esterified) CO2H, trihalomethyl, R3 = substituted aryl or heterocyclyl] are prepared, e.g. by reaction of R3COCH2COR2, OHCCHR3COR2, or OHCCHR2COR3 with R1NHNH2. Thus, a mixture of Et 4-(4-methylthiophenyl)-2,4-dioxobutanoate and 4-FC6H4NHNH2.HCl in EtOH-dioxane was refluxed 5 h to give Et 1-(4-fluorophenyl)-3-(4-methylthiophenyl)pyrazole-5-carboxylate. A total of approx. 250 I were prepared and 9 I at 3.2 or 10 mg/kg/day p.o. for 23 days inhibited 80.6-100% of mycobacterial adjuvant-induced secondary lesion in rat hind paws.

ST arylhydrazine cyclocondensation butanedione; pyrazole prepn antiinflammatory analgesic antithrombotic

IT Cyclocondensation reaction
(of arylhydrazines with butanediones, pyrazoles from)

IT **Analgesics**
Anticoagulants and Antithrombotics
Inflammation inhibitors
(pyrazole derivs.)

IT 134728-96-4P 134728-97-5P **134728-98-6P 134728-99-7P**
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134729-03-6P 134729-04-7P 134729-05-8P 134729-06-9P
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RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as antiinflammatory, analgesic, and antithrombotic)

IT **134731-30-9P** **134731-47-8P** 134753-97-2P 134753-98-3P
134753-99-4P 134754-00-0P 134754-01-1P **134754-02-2P**
134754-03-3P 134754-04-4P 134754-05-5P **134754-06-6P**
135327-58-1P
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as antiinflammatory, analgesic, and antithrombotic)

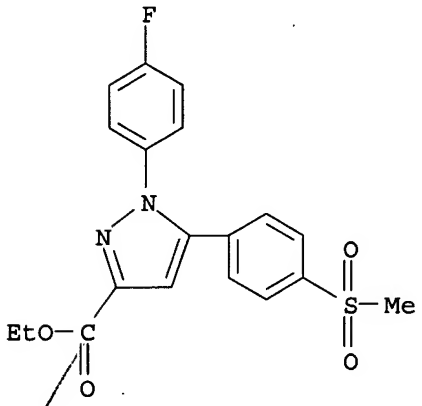
IT 24654-52-2P 56944-74-2P 119517-21-4P 126839-71-2P 134731-31-0P
134731-32-1P 134731-33-2P 134731-34-3P 134731-35-4P 134731-36-5P
134731-37-6P 134731-38-7P 134731-39-8P 134731-40-1P 134731-41-2P
134731-42-3P **134731-43-4P** **134731-44-5P** 134731-45-6P
134731-46-7P 134754-07-7P 134846-24-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, in preparation of antiinflammatory, analgesic, and antithrombotic pyrazole derivative)

IT 74-88-4, Iodomethane, reactions 74-89-5, Methylamine, reactions
75-36-5, Acetyl chloride 79-22-1, Methyl chloroformate 95-92-1, Diethyl oxalate 105-53-3, Diethyl malonate 108-24-7, Acetic anhydride
124-63-0, Methanesulfonyl chloride 364-78-3, 4-Fluoro-2-nitroaniline
371-14-2 506-59-2, Dimethylamine hydrochloride 544-92-3, Cuprous cyanide 823-85-8, 4-Fluorophenylhydrazine hydrochloride 1778-09-2
2537-48-6, Diethyl cyanomethylphosphonate 3446-89-7,
4-(Methylthio)benzaldehyde 5814-37-9 7664-41-7, Ammonia, reactions
26628-22-8, Sodium azide

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of antiinflammatory, analgesic, and antithrombotic pyrazole derivative)

IT **134728-98-6P**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as antiinflammatory, analgesic, and antithrombotic)

RN 134728-98-6 HCAPLUS
CN 1H-Pyrazole-3-carboxylic acid, 1-(4-fluorophenyl)-5-[4-(methylsulfonyl)phenyl]-, ethyl ester (9CI) (CA INDEX NAME)



L102 ANSWER 37 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN **1988:186735** HCAPLUS
DN **108:186735**
ED Entered STN: 28 May 1988
TI Preparation of 3-substituted 1,5-diphenylpyrazoles as antiinflammatories
IN Wachter, Michael Paul; Ferro, Michael Paul
PA Ortho Pharmaceutical Corp., USA
SO Eur. Pat. Appl., 50 pp.
CODEN: EPXXDW
DT Patent
LA English
IC ICM C07D231-12
ICS C07D403-12; C07D417-12; C07D401-12; A61K031-415; A61K031-425; A61K031-41
ICA C07C059-84; C07C059-88
CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI EP 248594	A2	19871209	EP 1987-304720	19870528 <--
EP 248594	A3	19881117		
EP 248594	B1	19931124		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
US 4826868	A	19890502	US 1987-42661	19870429 <--
DK 8702735	A	19871130	DK 1987-2735	19870527 <--
DK 170202	B1	19950612		
NO 8702228	A	19871130	NO 1987-2228	19870527 <--
NO 172236	B	19930315		
NO 172236	C	19930623		
AU 8773608	A1	19871210	AU 1987-73608	19870527 <--
AU 596844	B2	19900517		

ZA 8703842	A	19890125	ZA 1987-3842	19870527	<--
CA 1337122	A1	19950926	CA 1987-538137	19870527	<--
FI 8702379	A	19871130	FI 1987-2379	19870528	<--
FI 94340	B	19950515			
FI 94340	C	19950825			
AT 97660	E	19931215	AT 1987-304720	19870528	<--
ES 2059377	T3	19941116	ES 1987-304720	19870528	<--
HU 68247	A2	19950628	HU 1987-2466	19870528	<--
CN 87103953	A	19871209	CN 1987-103953	19870529	<--
CN 1028227	B	19950419			
JP 63022080	A2	19880129	JP 1987-134789	19870529	<--
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US 5164381	A	19921117	US 1991-730515	19910712	<--
PRAI US 1986-867996		19860529	<--		
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US 1989-339272		19890414	<--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
EP 248594	ICM	C07D231-12
	ICS	C07D403-12; C07D417-12; C07D401-12; A61K031-415; A61K031-425; A61K031-41
	ICA	C07C059-84; C07C059-88

OS CASREACT 108:186735

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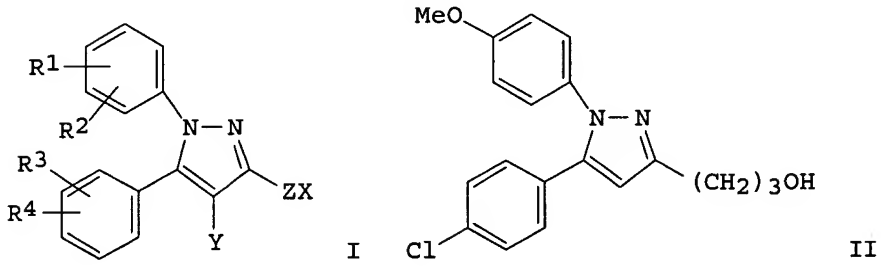

AB The title compds. [I; R1-R4 = H, alkoxy, Ph, halo, OH, alkylthio, alkylsulfonyl, NO2, CF3, amino, AcNH, CO2H, (un)substituted alkyl; R1R2, R3R4 = atoms to complete an (un)substituted benzo ring; X = (esterified) OH or CO2H, alkoxy, alkanoyl, acyl, amino, oximino, etc.; Y = H, alkyl, Br, Cl; Z = divalent, (un)substituted, (un)saturated C2-16 hydrocarbon residue] and their pharmaceutically acceptable salts were prepared as inflammation inhibitors. 4-ClC6H4COCH2CO(CH2)3OH was added to a mixture of 4-MeOC6H4NHNH2.HCl and pyridine in MeOH, and the resulting mixture stirred 1.5 h at room temperature to give 91% diphenylpyrazolepropanol II. In the rat paw edema test II had an ED50 of 3.6 mg/kg/day orally for 5 days.

ST phenylpyrazole prepn inflammation inhibitor; pyrazole diphenyl prepn antiinflammatory

IT **Allergy inhibitors**
Inflammation inhibitors
(diphenylpyrazoles)

IT **Dermatitis**
Psoriasis
(treatment of, diphenylpyrazoles for)

IT **Bronchodilators**
(**antiasthmatics**, diphenylpyrazoles)

IT Vasodilators
(coronary, diphenylpyrazoles)

IT Heart, disease or disorder

(infarction, treatment of, diphenylpyrazoles for)
IT Cardiotonics
(inotropics, diphenylpyrazoles)
IT Heart, disease or disorder
(ischemia, treatment of, diphenylpyrazoles for)
IT **39391-18-9, Cyclooxygenase 80619-02-9, 5-Lipoxygenase**
RL: RCT (Reactant); RACT (Reactant or reagent)
(inhibitors of, diphenylpyrazoles as)
IT 114151-49-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of pyrazole antiinflammatories)
IT 103475-41-8P 111881-78-8P 114149-85-8P 114149-86-9P 114149-87-0P
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RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as antiinflammatory)
IT 56-40-6, reactions 75-16-1, Methylmagnesium bromide 79-04-9
108-30-5, reactions 814-49-3, Diethyl chlorophosphate 1118-68-9, N,N-Dimethylglycine 1449-46-3, Benzyltriphenylphosphonium bromide 3282-30-2, Trimethylacetyl chloride 4229-44-1 4755-77-5, Ethyl oxalyl chloride 5470-11-1, Hydroxylamine hydrochloride 13266-02-9, Triphenyl(tridecyl)phosphonium bromide 17814-85-6, (4-Carboxybutyl)triphenylphosphonium bromide 19501-58-7, (4-Methoxyphenyl)hydrazine hydrochloride 30216-51-4, 2-Thiazolylhydrazine 57497-39-9, N-tert-Butylhydroxylamine hydrochloride 114151-48-3

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of pyrazole antiinflammatories)
IT **39391-18-9, Cyclooxygenase**
RL: **BAC (Biological activity or effector, except adverse)**; RACT (Reactant or reagent); **THU (Therapeutic use)**
(inhibitors of, diphenylpyrazoles as)
RN 39391-18-9 HCAPLUS
CN Synthetase, prostaglandin endoperoxide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

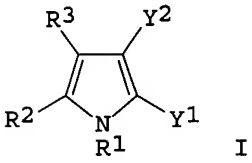
L102 ANSWER 38 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN **1987:213759** HCAPLUS
DN **106:213759**
ED Entered STN: 26 Jun 1987
TI Preparation and formulation of antiinflammatory 2-halo-4,5-diarylpyrroles
IN Wilkerson, Wendell W.
PA du Pont de Nemours, E. I., and Co., USA
SO U.S., 9 pp.
CODEN: USXXAM
DT Patent
LA English
IC A61K031-40; C07D207-34; C07D207-35; C07D207-416
NCL 514427000
CC 27-10 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 63
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 4652582	A	19870324	US 1985-690091	19850109 <--
PRAI US 1985-690091		19850109 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4652582	IC	A61K031-40IC C07D207-34IC C07D207-35IC C07D207-416
	NCL	514427000

OS CASREACT 106:213759
GI



I

AB Title compds. I (R1 = H, Me, Et, Ac, R4O2C, R4 = Me, Et, Me3C, PhCH2; R2, R3 = pyridyl, (un)substituted Ph; Y1 = halo; Y2 = H, Br, Cl) and their salts were prepared by 6 methods. Intermediates for I were also prepared I (R1, R2, R3 = H; Y1 = 4-MeSO2C6H4; Y2 = 4-FC6H4) in DMF was treated with N-chlorosuccinimide in DMF to give I (R1 = H; R2 = 4-FC6H4; R3 = 4-MeSO2C6H4; Y1 = Cl; Y2 = H) (II). II inhibited adjuvant-induced arthritis in rats with an ED50 of 0.5 mg/kg compared to 305 mg/kg for aspirin. Formulations of I are given.
ST halodiarylpyrrole prepn antiinflammatory pharmaceutical; pyrrole halodiaryl prepn antiinflammatory pharmaceutical
IT **Inflammation inhibitors**
(halodiarylpyrroles)
IT **Inflammation inhibitors**

(**antiarthritics**, halodiarylpyrroles)

IT **108381-57-3P 108400-78-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and bromination of)

IT **108381-58-4P 108381-59-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deprotection of, by alkaline hydrolysis)

IT **108381-60-8P 108381-61-9P 108381-62-0P**
108381-63-1P 108381-64-2P 108381-66-4P
108381-67-5P 108381-68-6P 108381-69-7P
108400-79-9P
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as antiinflammatory agent)

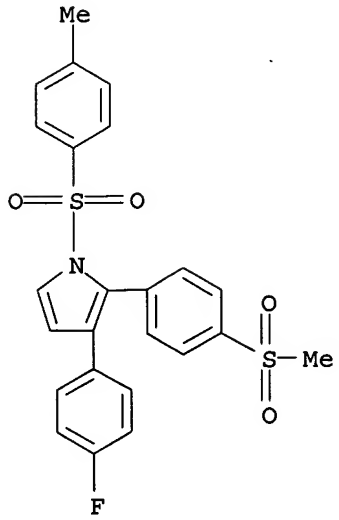
IT **78495-23-5**, 2-(4-Methylsulfonylphenyl)-3-(4-fluorophenyl)-1H-pyrrole
RL: RCT (Reactant); RACT (Reactant or reagent)
(protection and halogenation of)

IT 75-36-5 98-59-9, Toluenesulfonyl chloride 24424-99-5, Di-tert-butyl dicarbonate
RL: RCT (Reactant); RACT (Reactant or reagent)
(protection by, of pyrrole derivs.)

IT **108381-65-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution reaction of, with bromosuccinimide)

IT **108381-57-3P**
RL: **BAC (Biological activity or effector, except adverse)**; SPN (Synthetic preparation); PREP (Preparation); **THU (Therapeutic use)**
(preparation and bromination of)

RN 108381-57-3 HCAPLUS
CN 1H-Pyrrole, 3-(4-fluorophenyl)-1-[(4-methylphenyl)sulfonyl]-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)

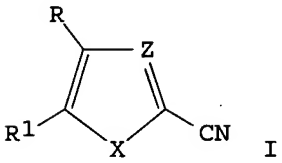


L102 ANSWER 39 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN **1987:49942** HCAPLUS
DN **106:49942**

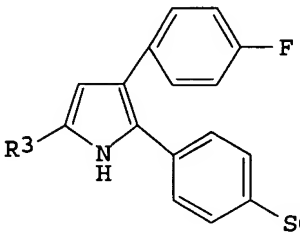
ED Entered STN: 21 Feb 1987
TI Antiinflammatory 2-cyano-4,5-diarylheterocycles
AU Wilkerson, W. W.
CS Biomed. Prod. Dep., E. I. du Pont de Nemours and Co., Wilmington, DE, 19898, USA
SO Research Disclosure (**1986**), 266, 323-4 (No. 26615)
CODEN: RSDSBB; ISSN: 0374-4353
DT Journal; Patent
LA English
CC 27-10 (Heterocyclic Compounds (One Hetero Atom))

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI RD 266015		19860610		
PRAI RD 1986-266015		**19860610**		

GI

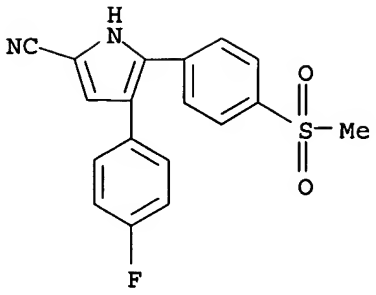


I



II

AB The title compds. I (X = NH, O, S; Z = CH, N; one of R and R1 = R2SOnC6H4 the other is Ph, substituted Ph; R2 = Me, Et; n = 0-2) were prepared Thus, the pyrrole II (R3 = H) was treated with ClSO2NCO to give II (R3 = cyano) which had one antiinflammatory ED53 of 1.3 mg/kg orally in the adjuvant arthritis test.
ST diarylpyrrolecarbonitrile prepn antiinflammatory; pyrrolecarbonitrile diaryl prepn antiinflammatory
IT **Inflammation inhibitors**
(diarylpyrrolecarbonitriles)
IT **106315-66-6P**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antiinflammatory activity of)
IT **78495-23-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chlorosulfonyl isocyanate)
IT **106315-66-6P**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antiinflammatory activity of)
RN 106315-66-6 HCAPLUS
CN 1H-Pyrrole-2-carbonitrile, 4-(4-fluorophenyl)-5-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



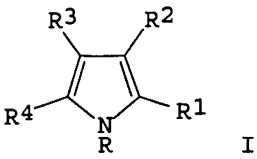
L102 ANSWER 40 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN **1985:113283** HCAPLUS
DN **102:113283**
ED Entered STN: 06 Apr 1985
TI Antiinflammatory and/or analgesic 1-alkyl-4,5-diaryl-2-fluoroalkyl-1H-pyrroles
IN Cherkofsky, Saul C.
PA du Pont de Nemours, E. I., and Co. , USA
SO U.S., 6 pp.
CODEN: USXXAM
DT Patent
LA English
IC C07D207-32; C01D403-04; A61K031-44; A61K031-40
NCL 424274000
CC 27-10 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 63
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 4477463	A	19841016	US 1982-376650	19820510 <--
PRAI US 1982-376650		19820510 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4477463	IC	C07D207-32IC C01D403-04IC A61K031-44IC A61K031-40
	NCL	424274000

OS CASREACT 102:113283
GI



I

AB Pyrroles I [R = Me, Et; R1 = CF3, C2F5; R2 = H, Me, Et; R3 and R4 are pyridyl, 4-R5C6H4 (R5 = H, F, Cl, Br, alkyl, alkylthio, alkylsulfonyl, alkoxy, dialkylamino)], which were prepared, exhibited analgesic and antiinflammatory activity. I (R = Me, R1 = R2 = H, R3 = R4 = 4-MeOC6H4) was heated with CF3I and EtN(CHMe2)2 at 150° to give I (R = Me, R1 = CF3, R2 = H, R3 = R4 = 4-MeOC6H4).
ST fluoroalkylpyrrole prepn analgesic antiinflammatory; pyrrole fluoroalkyl prepn antiinflammatory
IT **Analgesics**

Inflammation inhibitors and Antiarthritics
((perfluoroalkyl)pyrroles)

IT 2314-97-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkylation by, of N-methylpyrrole derivative)

IT 95037-07-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and alkylation of, by trifluoromethyl iodide)

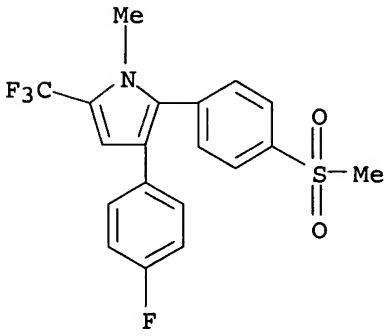
IT 95037-08-4P 95037-09-5P 95037-10-8P 95037-11-9P **95037-12-0P** 95037-13-1P 95050-60-5P 95050-61-6P
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and analgesic and antiinflammatory activity of)

IT 74-88-4, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(N-alkylation by, of pyrrole derivative)

IT 5834-50-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(N-methylation of)

IT **95037-12-0P**
RL: **BAC (Biological activity or effector, except adverse)**; BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and analgesic and antiinflammatory activity of)

RN 95037-12-0 HCAPLUS
CN 1H-Pyrrole, 3-(4-fluorophenyl)-1-methyl-2-[4-(methylsulfonyl)phenyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L102 ANSWER 41 OF 41 HCAPLUS COPYRIGHT 2004 ACS on STN
AN **1970:100495** HCAPLUS
DN **72:100495**
ED Entered STN: 12 May 1984
TI 1-Phenylpyrroles
IN Pons, Andre L.; Robba, Max F.; Marcy, Rene H.; Duval, Denise J. C.
PA Innothera
SO Ger. Offen., 94 pp.
CODEN: GWXXBX
DT Patent
LA German
IC C07D; A61K
CC 27 (Heterocyclic Compounds (One Hetero Atom))
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

PI	DE 1938904	A	19700205	DE 1969-1938904	19690731 <--
	FR 7649	M	19700202	FR 1968-161664	19680802 <--
	FR 2054474	A6	19710423	FR 1969-23303	19690709 <--
	FR 2054474	B2	19730608		
	GB 1263940	A	19720216	GB 1969-1263940	19690731 <--
PRAI	FR 1968-161664		19680802 <--		
	FR 1969-23303		19690709 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
DE 1938904	IC	C07DIC A61K

GI For diagram(s), see printed CA Issue.

AB 1-Phenylpyrroles (I) are prepared and investigated as pain killers and inflammation inhibitors for the treatment of arthritis, lumbago, and sciatica, Thus, 33 g γ-oxovalerophenone and 25 g m-aminobenzoic acid was heated at 195° to yield 95% I (R = m-CO2H, R1 = Me, R2 = Ph), m. 197° (EtOH), LD50 (mg/kg in mice) i.v. 113, i.p. 430, and digestive 1850. Ninety I were prepared and the LD50 determined for 20.

ST analgesic phenyl pyrroles; phenyl pyrroles analgesic; pyrroles phenyl analgesic; antiinflammatory phenyl pyroles

IT **Analgesics**
(phenylpyrrole derivs.)

IT Benzoic acid, m-[2-(p-bromophenyl)-5-methylpyrrol-1-yl]-
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 853-37-2P 15898-26-7P 26165-49-1P 26165-50-4P 26165-51-5P
26165-52-6P 26165-53-7P 26165-54-8P 26165-55-9P 26165-56-0P
26165-57-1P 26165-58-2P 26165-61-7P 26165-62-8P 26165-63-9P
26165-64-0P 26165-65-1P 26165-66-2P 26165-67-3P 26165-68-4P
26165-69-5P 26165-70-8P **26165-71-9P** 26165-72-0P
26165-73-1P 26165-74-2P 26165-75-3P 26165-76-4P 26165-77-5P
26165-78-6P 26165-79-7P 26165-80-0P 26165-81-1P 26165-82-2P
26165-83-3P 26165-84-4P 26165-85-5P 26165-86-6P 26165-88-8P
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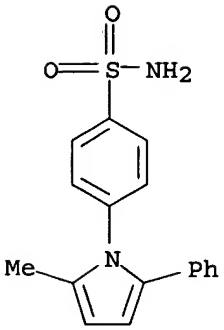
26180-33-6P 26180-34-7P 26180-35-8P 26180-36-9P 26180-37-0P
26180-38-1P 26180-40-5P 26180-41-6P 26180-42-7P 26180-43-8P
26180-44-9P 26180-45-0P 26180-46-1P 26180-47-2P 26180-48-3P
26180-49-4P 26180-50-7P 26180-51-8P 26180-52-9P 26180-53-0P
26180-54-1P 26180-55-2P 26180-56-3P 26180-57-4P 26180-58-5P
26180-59-6P 26180-60-9P 26180-61-0P 26180-62-1P 26180-63-2P
26180-64-3P 26180-65-4P 26180-66-5P 26180-67-6P 26281-26-5P
26281-27-6P 26281-28-7P 26281-29-8P 26281-30-1P 26342-77-8P
27766-51-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT **26165-71-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 26165-71-9 HCAPLUS

CN Benzenesulfonamide, p-(2-methyl-5-phenylpyrrol-1-yl)- (8CI) (CA INDEX NAME)



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FILE 'REGISTRY' ENTERED AT 16:38:35 ON 20 OCT 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 19 OCT 2004 HIGHEST RN 765878-56-6
DICTIONARY FILE UPDATES: 19 OCT 2004 HIGHEST RN 765878-56-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

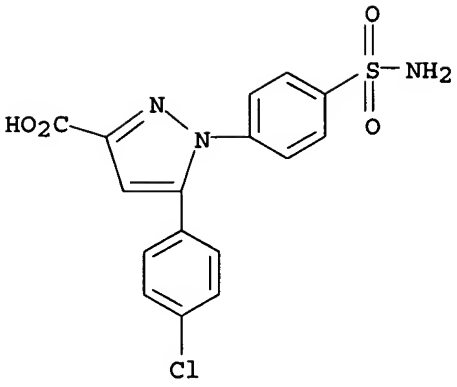
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> d scan l35

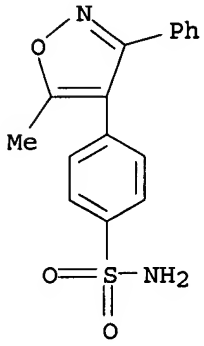
L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Pyrazole-3-carboxylic acid, 1-[4-(aminosulfonyl)phenyl]-5-(4-chlorophenyl)- (9CI)
MF **C16 H12 Cl N3 O4 S**



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

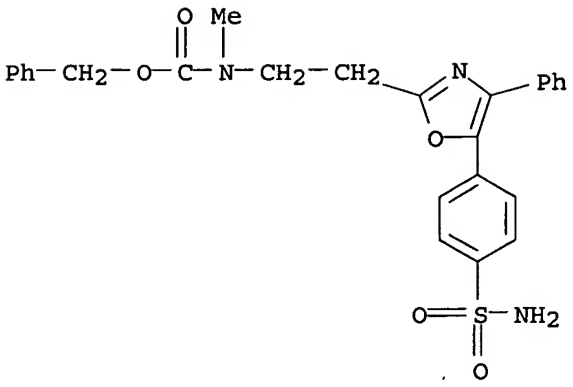
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):45

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-(5-methyl-3-phenyl-4-isoxazolyl)- (9CI)
MF **C16 H14 N2 O3 S**
CI COM



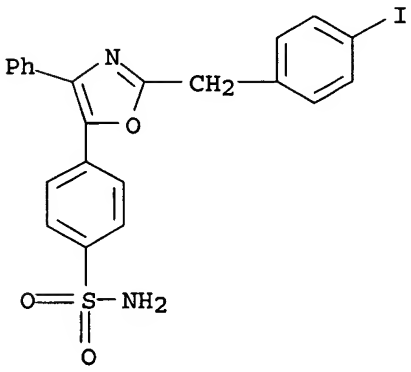
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Carbamic acid, [2-[5-[4-(aminosulfonyl)phenyl]-4-phenyl-2-oxazolyl]ethyl]methyl-, phenylmethyl ester (9CI)
MF **C26 H25 N3 O5 S**



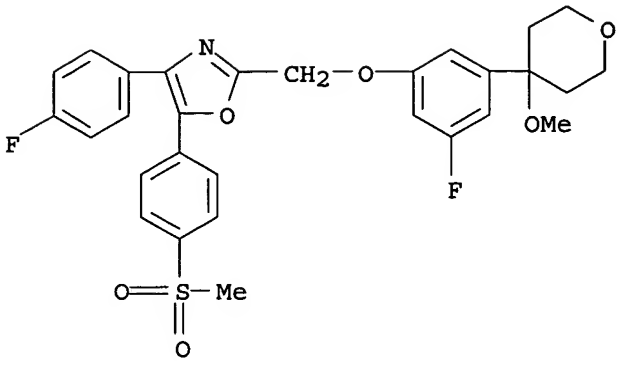
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[2-[(4-iodophenyl)methyl]-4-phenyl-5-oxazolyl]- (9CI)
MF **C22 H17 I N2 O3 S**



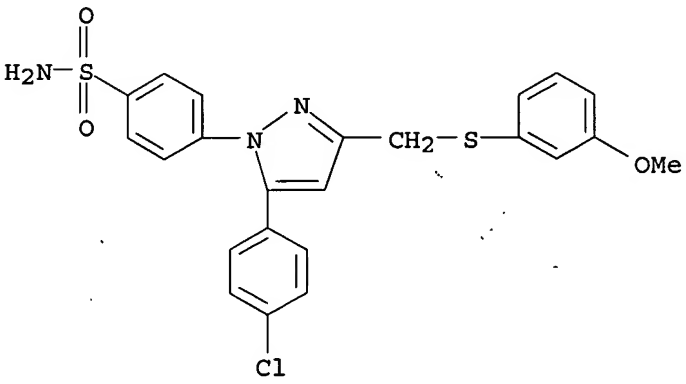
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

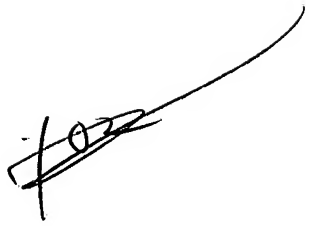
L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Oxazole, 4-(4-fluorophenyl)-2-[[3-fluoro-5-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenoxy]methyl]-5-[4-(methylsulfonyl)phenyl]- (9CI)
MF **C29 H27 F2 N O6 S**



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

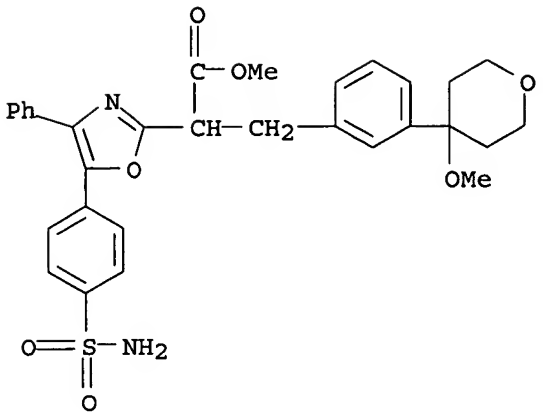
L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[5-(4-chlorophenyl)-3-[[(3-methoxyphenyl)thio]methyl]-1H-pyrazol-1-yl]- (9CI)
MF **C23 H20 Cl N3 O3 S2**





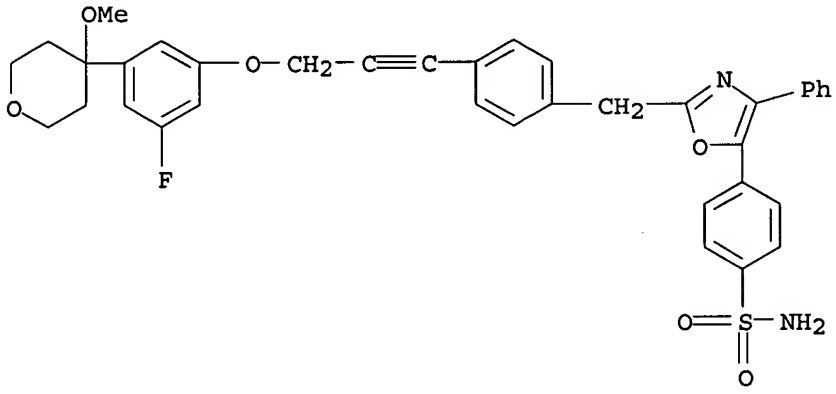
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2-Oxazoleacetic acid, 5-[4-(aminosulfonyl)phenyl]-4-phenyl-α-[[3-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenyl]methyl]-, methyl ester (9CI)
MF **C31 H32 N2 O7 S**



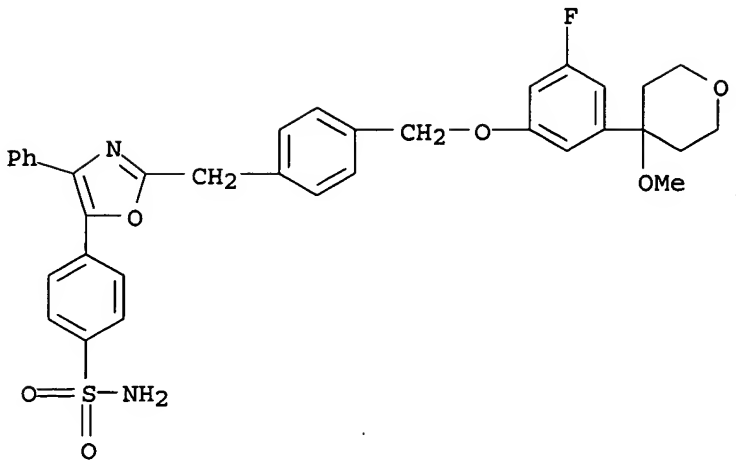
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[2-[[4-[3-[3-fluoro-5-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenoxy]-1-propynyl]phenyl]methyl]-4-phenyl-5-oxazolyl]- (9CI)
MF **C37 H33 F N2 O6 S**



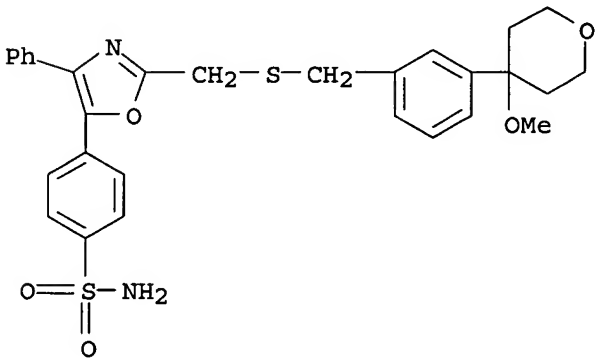
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[2-[[4-[[3-fluoro-5-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenoxy]methyl]phenyl]methyl]-4-phenyl-5-oxazolyl]- (9CI)
MF **C35 H33 F N2 O6 S**



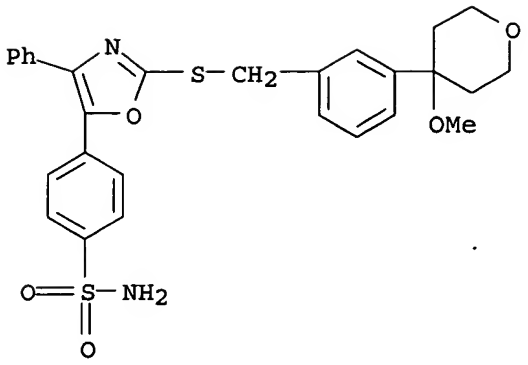
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[4-phenyl-2-[[[[3-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenyl]methyl]thio]methyl]-5-oxazolyl]- (9CI)
MF **C29 H30 N2 O5 S2**



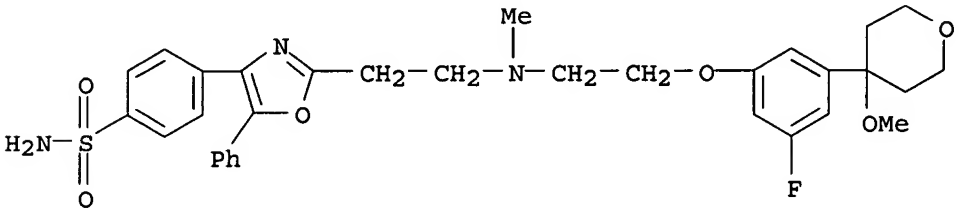
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[4-phenyl-2-[[[3-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenyl]methyl]thio]-5-oxazolyl]- (9CI)
MF **C28 H28 N2 O5 S2**



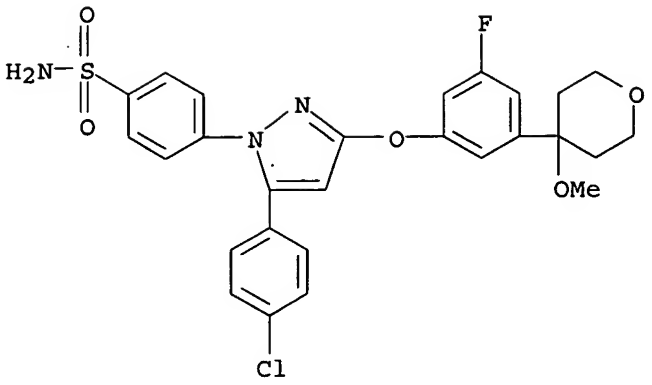
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[2-[2-[[2-[3-fluoro-5-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenoxy]ethyl]methylamino]ethyl]-5-phenyl-4-oxazolyl]- (9CI)
MF **C32 H36 F N3 O6 S**
CI COM



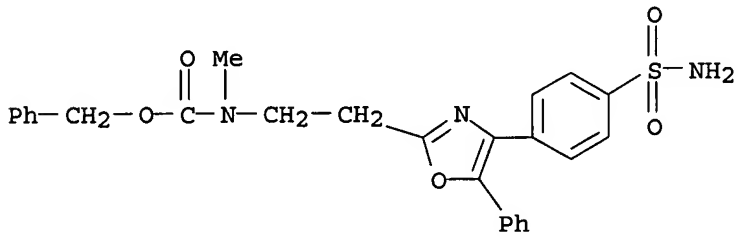
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[5-(4-chlorophenyl)-3-[3-fluoro-5-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenoxy]-1H-pyrazol-1-yl]- (9CI)
MF **C27 H25 Cl F N3 O5 S**



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

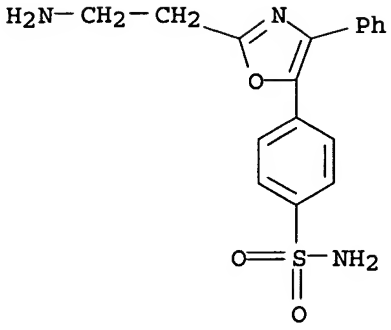
L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Carbamic acid, [2-[4-[4-(aminosulfonyl)phenyl]-5-phenyl-2-oxazolyl]ethyl]methyl-, phenylmethyl ester (9CI)
MF **C26 H25 N3 O5 S**



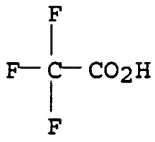
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[2-(2-aminoethyl)-4-phenyl-5-oxazolyl]-, mono(trifluoroacetate) (9CI)
MF **C17 H17 N3 O3 S . C2 H F3 O2**

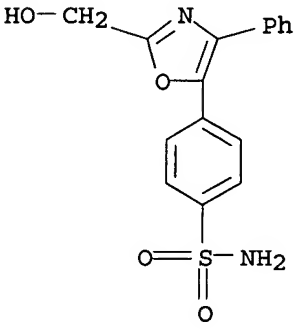
CM 1



CM 2

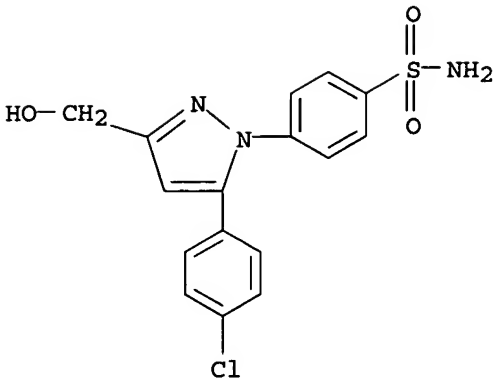


L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[2-(hydroxymethyl)-4-phenyl-5-oxazolyl]- (9CI)
MF **C16 H14 N2 O4 S**



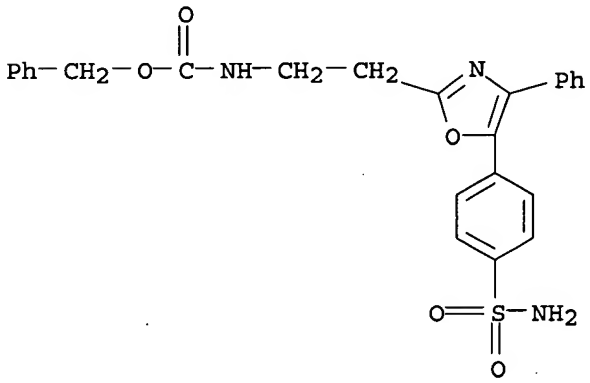
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[5-(4-chlorophenyl)-3-(hydroxymethyl)-1H-pyrazol-1-yl]- (9CI)
MF **C16 H14 Cl N3 O3 S**



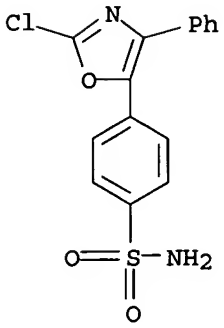
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Carbamic acid, [2-[5-[4-(aminosulfonyl)phenyl]-4-phenyl-2-oxazolyl]ethyl]-, phenylmethyl ester (9CI)
MF **C25 H23 N3 O5 S**



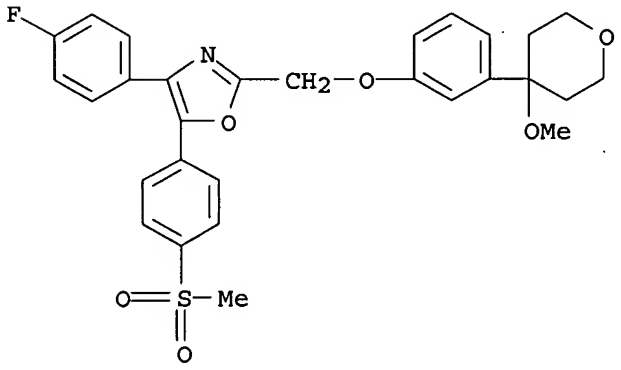
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-(2-chloro-4-phenyl-5-oxazolyl)- (9CI)
MF **C15 H11 Cl N2 O3 S**



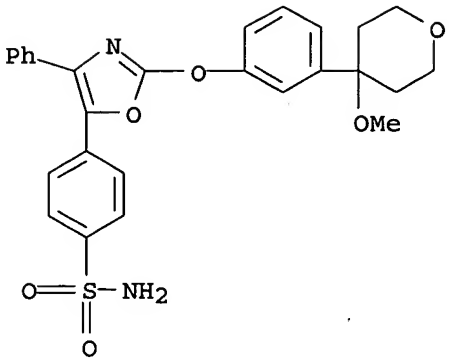
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Oxazole, 4-(4-fluorophenyl)-5-[4-(methylsulfonyl)phenyl]-2-[[3-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenoxy]methyl]- (9CI)
MF **C29 H28 F N O6 S**



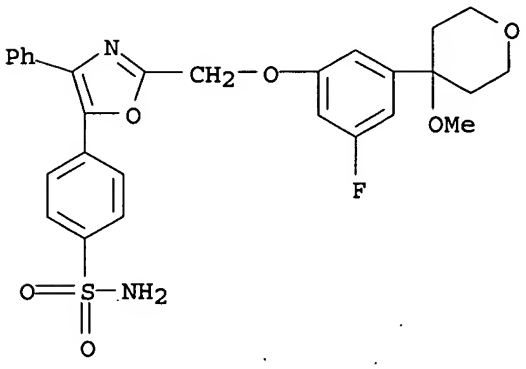
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[4-phenyl-2-[3-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenoxy]-5-oxazolyl]- (9CI)
MF **C27 H26 N2 O6 S**



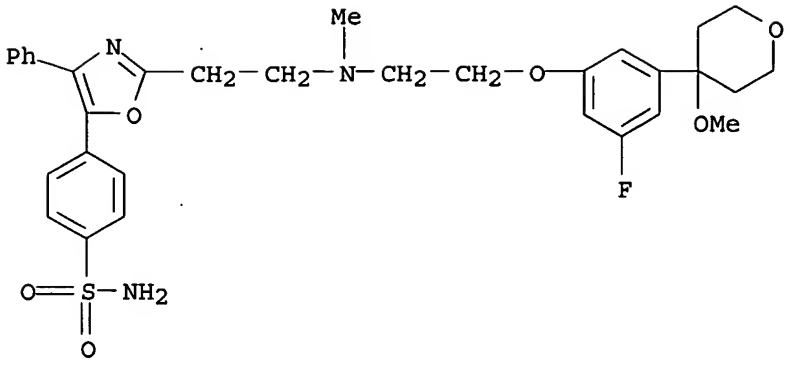
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[2-[[3-fluoro-5-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenoxy]methyl]-4-phenyl-5-oxazolyl]- (9CI)
MF **C28 H27 F N2 O6 S**



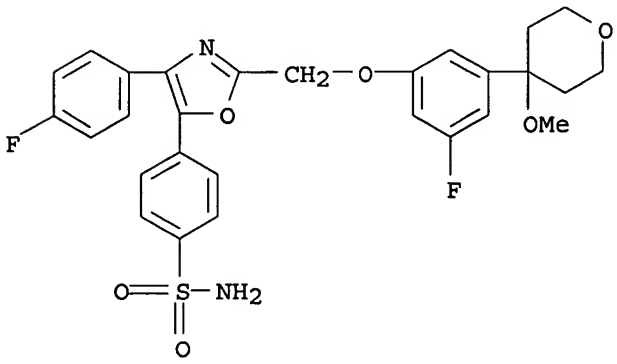
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[2-[2-[[2-[3-fluoro-5-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenoxy]ethyl]methylamino]ethyl]-4-phenyl-5-oxazolyl]- (9CI)
MF **C32 H36 F N3 O6 S**
CI COM



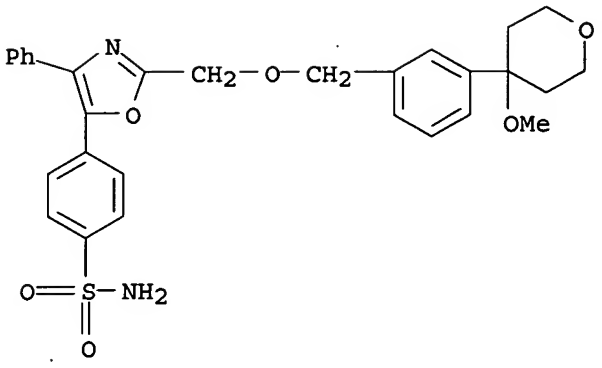
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[4-(4-fluorophenyl)-2-[[3-fluoro-5-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenoxy]methyl]-5-oxazolyl]- (9CI)
MF **C28 H26 F2 N2 O6 S**



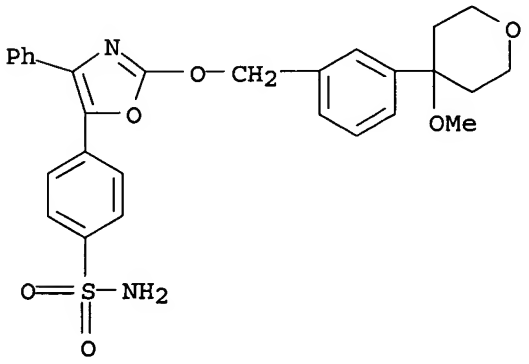
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[4-phenyl-2-[[[3-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenyl]methoxy]methyl]-5-oxazolyl]- (9CI)
MF **C29 H30 N2 O6 S**



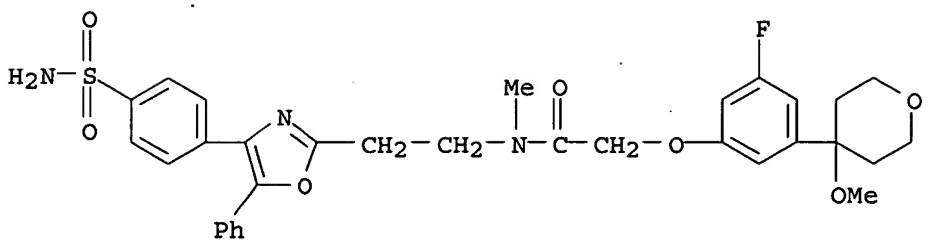
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[4-phenyl-2-[[3-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenyl]methoxy]-5-oxazolyl]- (9CI)
MF **C28 H28 N2 O6 S**



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

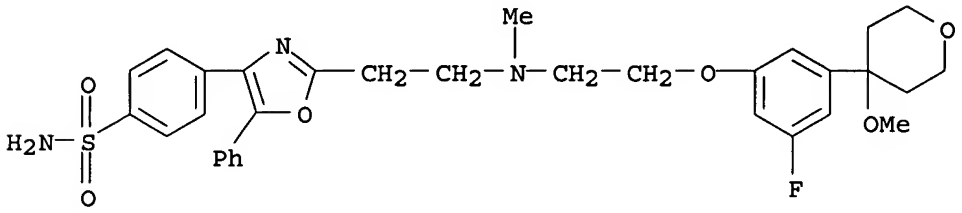
L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Acetamide, N-[2-[4-[4-(aminosulfonyl)phenyl]-5-phenyl-2-oxazolyl]ethyl]-2-[3-fluoro-5-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenoxy]-N-methyl- (9CI)
MF **C32 H34 F N3 O7 S**



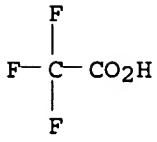
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[2-[2-[[2-[3-fluoro-5-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenoxy]ethyl]methylamino]ethyl]-5-phenyl-4-oxazolyl]-, mono(trifluoroacetate) (9CI)
MF **C32 H36 F N3 O6 S . C2 H F3 O2**

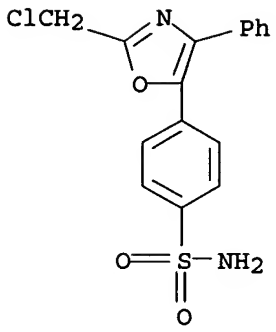
CM 1



CM 2



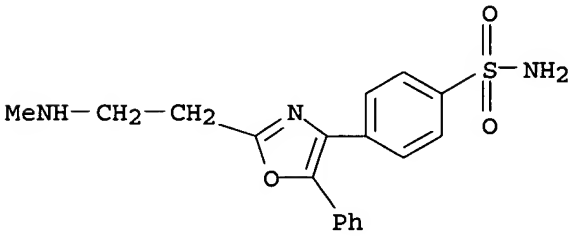
L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[2-(chloromethyl)-4-phenyl-5-oxazolyl]- (9CI)
MF **C16 H13 Cl N2 O3 S**



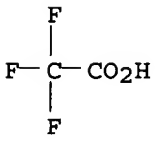
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[2-[2-(methylamino)ethyl]-5-phenyl-4-oxazolyl]-, mono(trifluoroacetate) (9CI)
MF **C18 H19 N3 O3 S . C2 H F3 O2**

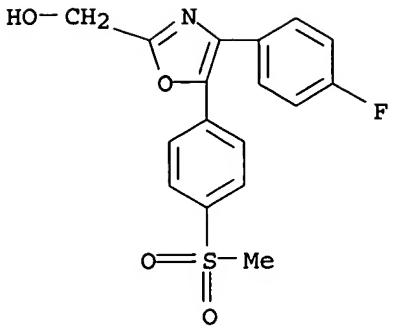
CM 1



CM 2

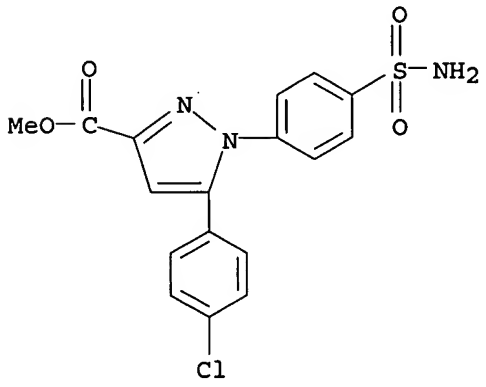


L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2-Oxazolemethanol, 4-(4-fluorophenyl)-5-[4-(methylsulfonyl)phenyl]- (9CI)
MF **C17 H14 F N O4 S**



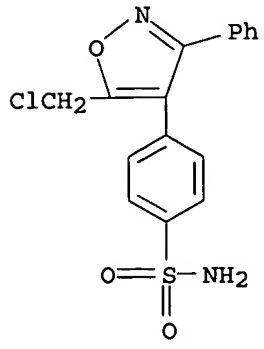
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Pyrazole-3-carboxylic acid, 1-[4-(aminosulfonyl)phenyl]-5-(4-chlorophenyl)-, methyl ester (9CI)
MF **C17 H14 Cl N3 O4 S**



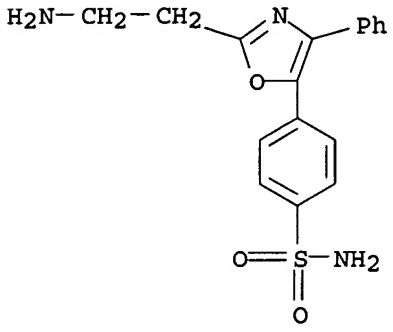
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[5-(chloromethyl)-3-phenyl-4-isoxazolyl]- (9CI)
MF **C16 H13 Cl N2 O3 S**



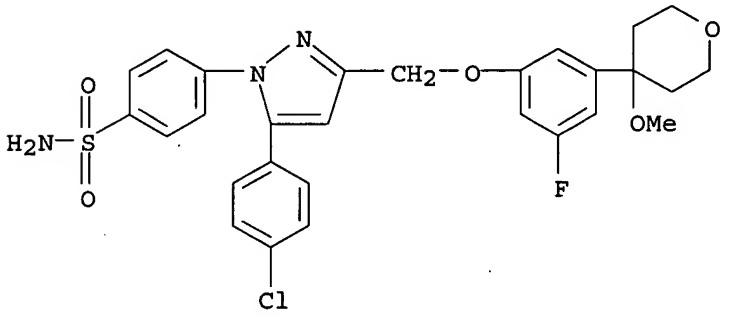
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[2-(2-aminoethyl)-4-phenyl-5-oxazolyl]- (9CI)
MF **C17 H17 N3 O3 S**
CI COM



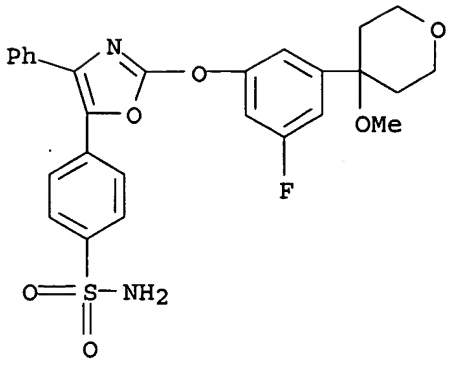
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[5-(4-chlorophenyl)-3-[[3-fluoro-5-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenoxy]methyl]-1H-pyrazol-1-yl]- (9CI)
MF **C28 H27 Cl F N3 O5 S**



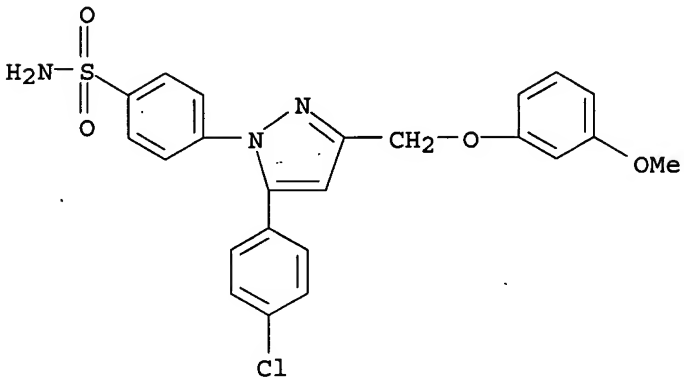
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[2-[3-fluoro-5-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenoxy]-4-phenyl-5-oxazolyl]- (9CI)
MF **C27 H25 F N2 O6 S**



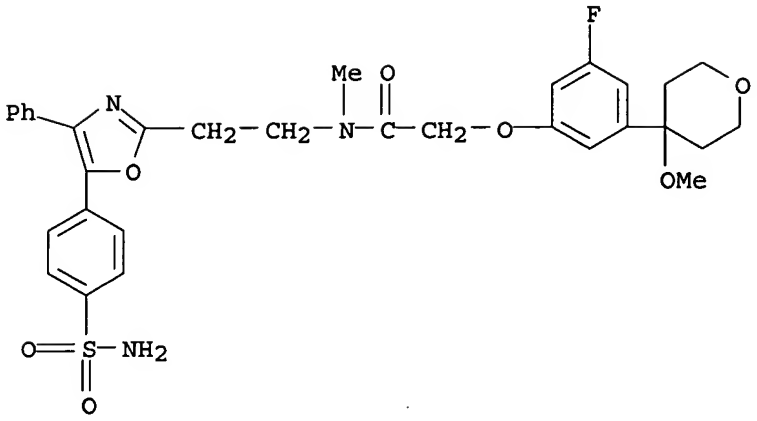
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[5-(4-chlorophenyl)-3-[(3-methoxyphenoxy)methyl]-1H-pyrazol-1-yl]- (9CI)
MF **C23 H20 Cl N3 O4 S**



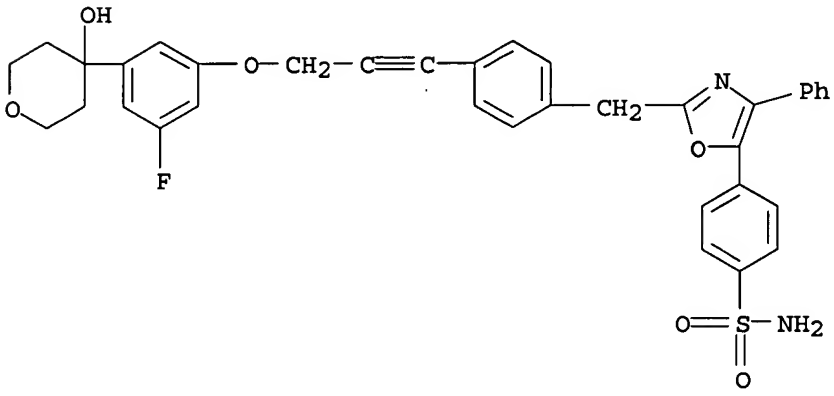
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Acetamide, N-[2-[5-[4-(aminosulfonyl)phenyl]-4-phenyl-2-oxazolyl]ethyl]-2-[3-fluoro-5-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenoxy]-N-methyl- (9CI)
MF **C32 H34 F N3 O7 S**



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[2-[[4-[3-[3-fluoro-5-(tetrahydro-4-hydroxy-2H-pyran-4-yl)phenoxy]-1-propynyl]phenyl]methyl]-4-phenyl-5-oxazolyl]- (9CI)
MF **C36 H31 F N2 O6 S**



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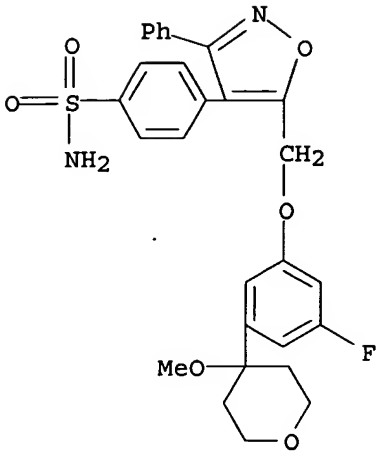
IN Benzenesulfonamide, 4-[5-[[3-fluoro-5-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenoxy]methyl]-3-phenyl-4-isoxazolyl]- (9CI)
MF **C28 H27 F N2 O6 S**



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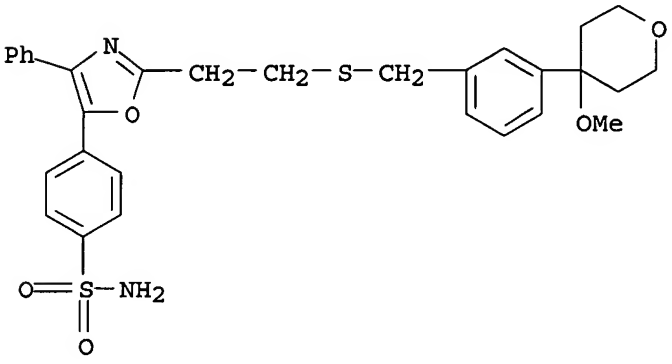
L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[4-phenyl-2-[2-[[[3-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenyl]methyl]thio]ethyl]-5-oxazolyl]- (9CI)
MF **C30 H32 N2 O5 S2**



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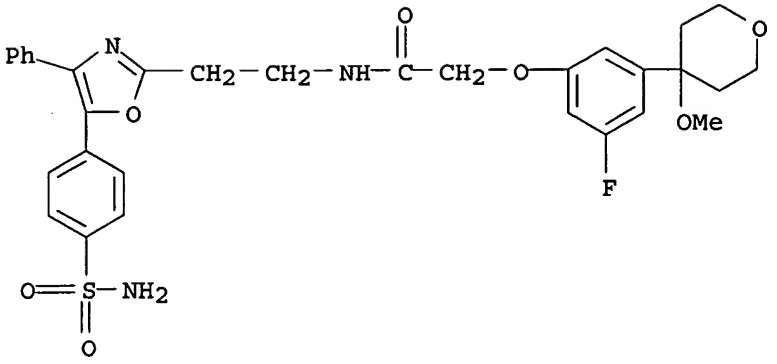
L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Acetamide, N-[2-[5-[4-(aminosulfonyl)phenyl]-4-phenyl-2-oxazolyl]ethyl]-2-[3-fluoro-5-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenoxy]- (9CI)
MF **C31 H32 F N3 O7 S**



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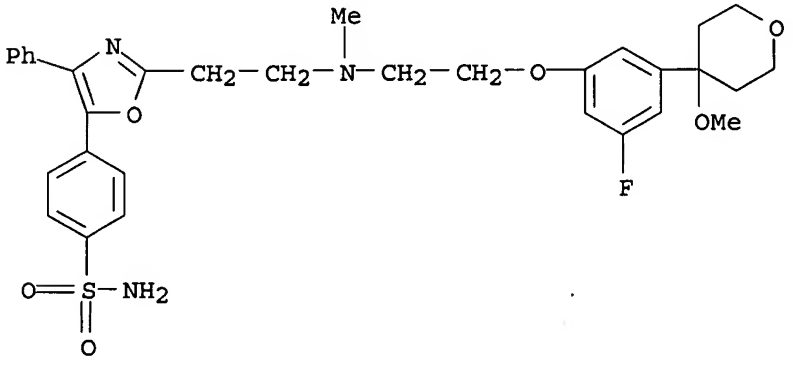
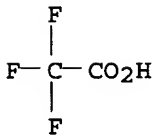
L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[2-[2-[[2-[3-fluoro-5-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenoxy]ethyl]methylamino]ethyl]-4-phenyl-5-oxazolyl]-, mono(trifluoroacetate) (9CI)
MF **C32 H36 F N3 O6 S . C2 H F3 O2**

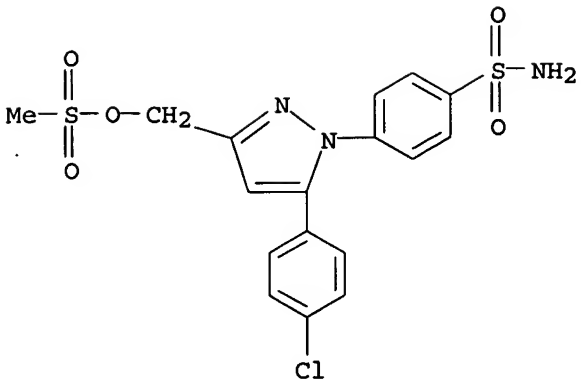
CM 1



CM 2



L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[5-(4-chlorophenyl)-3-[[(methylsulfonyl)oxy]methyl]-1H-pyrazol-1-yl]- (9CI)
MF **C17 H16 Cl N3 O5 S2**



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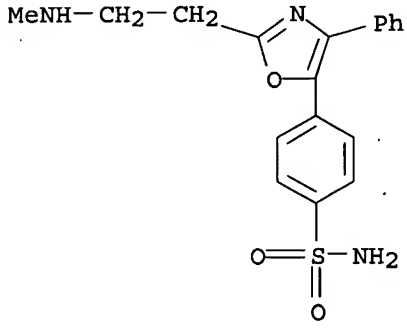
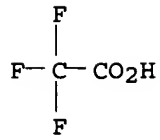
L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzenesulfonamide, 4-[2-[2-(methylamino)ethyl]-4-phenyl-5-oxazolyl]-, mono(trifluoroacetate) (9CI)
MF **C18 H19 N3 O3 S . C2 H F3 O2**

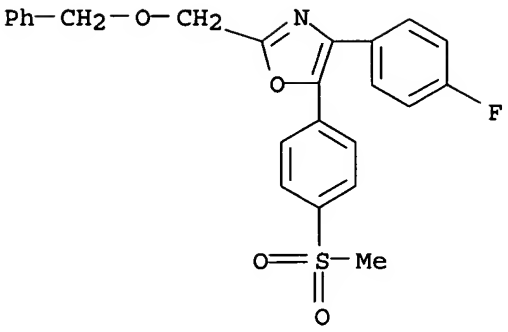
CM 1



CM 2



L35 46 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Oxazole, 4-(4-fluorophenyl)-5-[4-(methylsulfonyl)phenyl]-2-[(phenylmethoxy)methyl]- (9CI)
MF **C24 H20 F N O4 S**



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ALL ANSWERS HAVE BEEN SCANNED

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